Weierstraß-Institut
für Angewandte Analysis und Stochastik
Leibniz-Institut im Forschungsverbund Berlin e. V.

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An electronic model for solar cells including active interfaces and energy resolved defect densities

Annegret Glitzky

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Weierstrass Institute
Mohrenstr. 39
10117 Berlin
Germany
E-Mail: Annegret.Glitzky@wias-berlin.de

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Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

We introduce an electronic model for solar cells taking into account heterostructures with active interfaces and energy resolved volume and interface trap densities. The model consists of continuity equations for electrons and holes with thermionic emission transfer conditions at the interface and of ODEs for the trap densities with energy level and spatial position as parameters, where the right hand sides contain generation-recombination as well as ionization reactions. This system is coupled with a Poisson equation for the electrostatic potential.

We show the thermodynamic correctness of the model and prove a priori estimates for the solutions to the evolution system. Moreover, existence and uniqueness of weak solutions of the problem are proven. For this purpose we solve a regularized problem and verify bounds of the corresponding solution not depending on the regularization level.

1 Introduction and notation

The paper is devoted to the analysis of electronic models for solar cells including active interfaces, which take into account energy resolved defect (trap) densities. Different kinds of such traps occur in the bulk material and others live only at interfaces. These traps are assumed to be immobile, but during the time being they can change their charge states by reactions with bulk electrons and holes from both sides of the interface. Additionally thermionic emission effects for electrons and holes at the interface are taken into account.

Semiconductor models with varying in time densities of ionized impurities, where the impurities are associated to a fixed energy level have been investigated in [12]. Recently, in [9], we investigated a model with energy resolved defect densities in the bulk. But there no active interfaces (and no traps at interfaces) where taken into account.

Our equations are based on models proposed by engineers working on solar cells (see e.g. [20, Sect. 4.2]). But, for an easier writing we consider here the situation of only one kind of volume defects and one kind of interface defects. We demonstrate on this example how such defects can be analytically treated. Since there is only a very weak coupling of the effects of the different defects our ideas can easily be generalized to any finite number of kinds of defects in the bulk and at interfaces.

Moreover, we study here a special geometric situation of a heterostructure, which can be generalized to more complicated geometries. $\Omega \subset \mathbb{R}^2$ denotes the solar cell domain. The boundary $\partial\Omega$ of Ω splits up into a part Γ_D, representing the contacts of the device and a part Γ_N, where the device is insulated. Let a hypersurface Γ representing the active interface divide Ω into the two parts Ω^α and Ω^β (see Figure 1, too). We assume that the active interface Γ and the part of $\partial\Omega$, where Dirichlet conditions are prescribed, are strictly separated, that means $\inf_{x\in\Gamma_D,\, y\in\Gamma} |x-y| \geq \kappa_0 > 0$. We denote $\Gamma_D^\gamma = \Gamma_D \cap \overline{\Omega^\gamma}$, $\Gamma_N^\gamma = \partial\Omega^\gamma \setminus (\overline{\Gamma} \cup \overline{\Gamma_D})$, $\gamma = \alpha, \beta$. Note that Γ_D^γ is allowed to be empty for one γ.

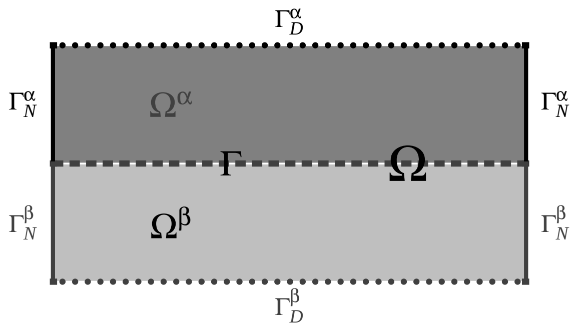

Figure 1: Heterostructure Ω with interface Γ.

For the analysis we rescale the quantities, such that energies are counted in units of k_BT, where k_B is Boltzmann's constant and T is the temperature. In this energy scale for $E \in E_G = [E_1, E_2]$ we take into account one kind of bulk (volume) defects with given defect distribution $N(x,E)$. To include also measure valued distributions of traps on the energy scale we use a finite nonnegative measure $\mu = N\mathrm{d}E$ on $G := \Omega \times E_G$ proposing Young measure type properties such that $\mu(x,\cdot)$ is a Radon measure on E_G a.e. on Ω and $x \mapsto \int_{E_G} g(E)\mu(x,\mathrm{d}E)$ is measurable for all continuous functions $g : E_G \to \mathbb{R}$.

This setting allows for $\mu(x,\cdot) = \sum_{k=1}^K \theta_k(x)\delta_{E_k(x)}(\cdot)$ such that the case of point-like distributed traps at single energies $E_{trap} \in E_G$ as discussed in [12] result as special case of our investigations, too.

Additionally we consider one type of interface defects with distribution $N_\Gamma(x,E)$. Similarly we work with a finite nonnegative measure $\mu_\Gamma = N_\Gamma \mathrm{d}E$ on $G_\Gamma := \Gamma \times E_G$.

We use the abbreviations

$$\langle\langle g\rangle\rangle := \int_{E_G} g(E)\mu(x,\mathrm{d}E), \quad \langle\langle g\rangle\rangle_\Gamma := \int_{E_G} g(E)\mu_\Gamma(x,\mathrm{d}E).$$

Besides the densities of electrons u_1 and holes u_2 depending only on the spatial position x we have to balance the following quantities: The probability that defect states with defect distribution $N(x,E)$ are occupied by an electron can be interpreted as the density of defects occupied by electrons on $G = \Omega \times E_G$ with respect to the measure μ. We denote it by u_3, and $u_4 = 1 - u_3$ corresponds to the density of non occupied defect states with respect to the measure μ. Correspondingly we denote the density of interfacial defects occupied by electrons on $G_\Gamma = \Gamma \times E_G$ with respect to the measure μ_Γ by $u_{\Gamma 1}$, and $u_{\Gamma 2} = 1 - u_{\Gamma 1}$ corresponds to the density of non occupied defect states with respect to the measure μ_Γ.

Moreover, we introduce the charge numbers of electrons, holes, volume and interface traps

$$\lambda_1 = -1, \quad \lambda_2 = 1, \quad \lambda_3 = \begin{cases} -1 & \text{for acceptor like traps} \\ 0 & \text{for donator like traps} \end{cases}, \quad \lambda_4 = \lambda_3 + 1,$$

$$\lambda_{\Gamma 1} = \begin{cases} -1 & \text{for acceptor like traps} \\ 0 & \text{for donator like traps} \end{cases}, \quad \lambda_{\Gamma 2} = \lambda_{\Gamma 1} + 1,$$

and use the vector $\lambda = (\lambda_1, \dots, \lambda_4, \lambda_{\Gamma 1}, \lambda_{\Gamma 2}) \in \mathbb{R}^6$. In the bulk we consider capture/escape reactions of electrons from the conduction band by unoccupied traps and of holes from the valence band by occupied traps (see R_1, R_2 in (1.5)). Also the interface defects capture and escape charge carriers from Ω^γ, see reaction rates R_1^Γ, R_2^Γ, $\gamma = \alpha, \beta$ in (1.5)).

The electronic model for solar cells with active interface proposed in [20] is a drift-diffusion model for the charge carriers coupled with ODEs for the defect occupation probabilities in the bulk $u_3(x,E)$, $u_4(x,E)$, $(x,E) \in G$ and with ODEs for the defect occupation probabilities at the interface $u_{\Gamma 1}(x,E)$, $u_{\Gamma 2}(x,E)$, $(x,E) \in G_\Gamma$. Additionally there occur transfer conditions at the interface including thermionic emission of electrons and holes. The incident light, generating pairs of electrons and holes is treated as a given (time dependent) source term G_{phot} in the continuity equations for electrons and holes. Let z denote the scaled electrostatic potential and let $u_i = (u_i^\alpha, u_i^\beta)$ be the carrier densities with u_i^γ being defined on $\overline{\Omega^\gamma}$, $\gamma = \alpha, \beta$, $i = 1, 2$. in our notation, the model proposed in [20, Sect. 4.2] can be written as the drift diffusion system

$$\begin{aligned} &-\nabla \cdot (\varepsilon \nabla z) = f - u_1 + u_2 + \sum_{i=3}^{4} \lambda_i \langle\langle u_i \rangle\rangle + \delta_\Gamma \sum_{i=1}^{2} \lambda_{\Gamma i} \langle\langle u_{\Gamma i} \rangle\rangle_\Gamma \quad \text{in } \mathbb{R}_+ \times \Omega, \\ &\frac{\partial}{\partial t} u_i^\gamma + \nabla \cdot j_i^\gamma = G_{phot} - R - \langle\langle R_i \rangle\rangle \quad \text{in } \mathbb{R}_+ \times \Omega^\gamma, \quad \gamma = \alpha, \beta, \ i = 1, 2, \end{aligned} \tag{1.1}$$

the ODEs

$$\frac{\partial}{\partial t} u_3 = R_1 - R_2, \quad \frac{\partial}{\partial t} u_4 = -\frac{\partial}{\partial t} u_3 \quad \text{on } \mathbb{R}_+ \times \operatorname{supp} \mu, \tag{1.2}$$

the ODEs at the interface

$$\frac{\partial}{\partial t} u_{\Gamma 1} = \sum_{\gamma = \alpha, \beta} \Big(R_{\Gamma 1}^\gamma - R_{\Gamma 2}^\gamma \Big), \quad \frac{\partial}{\partial t} u_{\Gamma 2} = -\frac{\partial}{\partial t} u_{\Gamma 1} \quad \text{on } \mathbb{R}_+ \times \operatorname{supp} \mu_\Gamma, \tag{1.3}$$

and the transfer conditions at the interface

$$\begin{aligned} &-j_i^\alpha \cdot \nu^\alpha = \sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta + \langle\langle R_{\Gamma i}^\alpha(\cdot, u_i^\alpha, u_{\Gamma 1}, u_{\Gamma 2}) \rangle\rangle_\Gamma, \\ &-j_i^\beta \cdot \nu^\beta = \sigma_i^\beta u_i^\beta - \sigma_i^\alpha u_i^\alpha + \langle\langle R_{\Gamma i}^\beta(\cdot, u_i^\beta, u_{\Gamma 1}, u_{\Gamma 2}) \rangle\rangle_\Gamma \quad \text{on } \mathbb{R}_+ \times \Gamma, \quad i = 1, 2. \end{aligned} \tag{1.4}$$

The flux terms and reaction rates in the continuity equations are given by

$$\begin{aligned} &j_i^\gamma = -D_i(\nabla u_i^\gamma + \lambda_i u_i^\gamma \nabla z), \quad \gamma = \alpha, \beta, \ i = 1, 2, \\ &R = R(u_1, u_2) = r_0(u_1, u_2)[u_1 u_2 - k_0], \\ &R_1 = R_1(E, u_1, u_3, u_4) = r_1[u_1 u_4 - k_1 u_3], \\ &R_2 = R_2(E, u_2, u_3, u_4) = r_2[u_2 u_3 - k_2 u_4], \\ &R_{\Gamma 1}^\gamma = R_{\Gamma 1}^\gamma(E, u_1^\gamma, u_{\Gamma 1}, u_{\Gamma 2}) = r_{\Gamma 1}^\gamma [u_1^\gamma u_{\Gamma 2} - k_{\Gamma 1}^\gamma u_{\Gamma 1}], \\ &R_{\Gamma 2}^\gamma = R_{\Gamma 2}^\gamma(E, u_2^\gamma, u_{\Gamma 1}, u_{\Gamma 2}) = r_{\Gamma 2}^\gamma [u_2^\gamma u_{\Gamma 1} - k_{\Gamma 2}^\gamma u_{\Gamma 2}], \end{aligned} \tag{1.5}$$

where the positive coefficients r_0, k_0 are allowed to depend in a nonsmooth way on the spatial position and the positive coefficients r_i, k_i, $r_{\Gamma i}^\gamma$, $k_{\Gamma i}^\gamma$, $\gamma = \alpha, \beta$, $i = 1, 2$, depend on (x, E). In the Poisson equation f means a fixed doping profile and δ_Γ denotes the surface measure on Γ such that in the sense of distributions $\int_\Omega w\delta_\Gamma v\,\mathrm{d}x = \int_\Gamma wv\,\mathrm{d}a$ for all test functions v.

For the Poisson equation on $\partial\Omega$ we suppose

$$z = z^D \text{ on } \mathbb{R}_+ \times \Gamma_D, \quad \nu \cdot (\varepsilon\nabla z) = 0 \text{ on } \mathbb{R}_+ \times \Gamma_N. \tag{1.6}$$

For the continuity equations for u_i^γ besides the transfer conditions (1.4) we assume that

$$u_i^\gamma = u_i^{\gamma D} \text{ on } \mathbb{R}_+ \times \Gamma_D^\gamma, \quad \nu \cdot j_i^\gamma = 0 \text{ on } \mathbb{R}_+ \times \Gamma_N^\gamma, \quad \gamma = \alpha, \beta, \; i = 1, 2. \tag{1.7}$$

We complete the model equations by initial conditions for the densities of all species

$$u_i(0) = U_i, \quad i = 1, \dots, 4, \quad u_{\Gamma i} = U_{\Gamma_i}, \quad i = 1, 2. \tag{1.8}$$

We introduce reference quantities $\widetilde{u}_3$, $\widetilde{u}_4$, $\widetilde{u}_{\Gamma 1}$, $\widetilde{u}_{\Gamma 2}$ fulfilling

$$u_1^D \widetilde{u}_4 = k_1 \widetilde{u}_3 \quad \mu\text{-a.e. in } G, \quad u_1^{\alpha D} \widetilde{u}_{\Gamma 2} = k_{\Gamma 1}^\alpha \widetilde{u}_{\Gamma 1} \quad \mu_\Gamma\text{-a.e. in } G_\Gamma.$$

Remark 1.1 *Our model is an extensive generalization of the classical van Roosbroeck system [21] describing charge transport in semiconductor devices due to drift and diffusion within a self-consistent electrical field. First mathematical analysis for this transient system was done in [18], for more references see [5]. Recently [22] investigated existence and asymptotic behavior of solutions for the whole space situation. Global existence and uniqueness of weak solutions under physically realistic conditions in two space dimensions is achieved in [6]. In [14] the van Roosbroeck system is reformulated as an evolution equation for the potentials. In this setting a unique, local in time solution in Lebesgue spaces is available and leads to classical solutions to the drift-diffusion equations in the two-dimensional case.*

To handle the electronic model for solar cells including active interfaces we profit from techniques approved for the van Roosbroeck system and combine them with new ideas.

The plan of the paper is the following: In Section 2 we collect our general assumptions and give a weak formulation (P) of the electronic model for solar cells including active interfaces. Section 3 is devoted to a priori estimates for solutions to (P). In Subsection 3.1 we start with energy estimates and we establish L^∞-estimates for solutions to (P) in Subsection 3.2. Section 4 contains the existence and uniqueness proof for (P). In Subsection 4.1 we introduce a regularized problem (P_M) and prove its solvability in Subsection 4.2. After deriving energy estimates (Subsection 4.3) and L^∞-estimates for solutions to (P_M) (Subsection 4.4) which are independent on the regularization level M, in Subsection 4.5 the existence and uniqueness result for (P) is shown.

2 Assumptions and weak formulation

2.1 Assumptions

Some notation. Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitzian domain. The notation of function spaces in the present paper corresponds to that in [15]. To specify norms, we write $\|\cdot\|_{L^p}$

and $\|\cdot\|_{H^1}$ instead of $\|\cdot\|_{L^p(\Omega)}$ and $\|\cdot\|_{H^1(\Omega)}$. Moreover, let Γ_N, Γ_D be disjoint open subsets of $\partial\Omega$ with $\partial\Omega = \overline{\Gamma_N} \cup \overline{\Gamma_D}$, where $\Gamma_0 := \overline{\Gamma_N} \cap \overline{\Gamma_D}$ consists of finitely many points. Let $\Omega \cup \Gamma_N$ be regular in the sense of Gröger [13]. For $1 \le p \le \infty$ we define $W_0^{1,p}(\Omega \cup \Gamma_N)$ as the closure of the set

$$\{w|_\Omega : w \in C^\infty(\mathbb{R}^2), (\Gamma_D \cup \Gamma_0) \cap \operatorname{supp}(w) = \emptyset\}$$

in $W^{1,p}(\Omega)$ equipped with the usual norm of the space $W^{1,p}(\Omega)$. Its dual is denoted by $W^{-1,p'}(\Omega \cup \Gamma_N)$, where $1/p + 1/p' = 1$, see [13]. Correspondingly we use $H_0^1(\Omega \cup \Gamma_N)$.

For a Banach space B we denote by B_+ the cone of non-negative elements and by B^* its dual space. We write u^+ (u^-) for the positive (negative) part of a function u. The abbreviation a.e. means $\mathcal{L}^d$-a.e., for the measures μ and μ_Γ we write μ-a.e. and μ_Γ-a.e. The scalar product in $\mathbb{R}^d$ is indicated by a centered dot. Positive constants which depend only on the data of our problem are denoted by c.

Now we collect the general assumptions our analytical investigations are based on.

(A1) Ω, Ω^α, $\Omega^\beta \subset \mathbb{R}^2$ are bounded Lipschitzian domains, Γ_D, Γ_N are disjoint open subsets of $\partial\Omega$, $\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_0$, mes $\Gamma_D > 0$, Γ_0 consists of finitely many points ($\Omega \cup \Gamma_N$ is regular in the sense of Gröger [13]).
A part Γ of a hypersurface devides Ω into Lipschitzian domains Ω^α and Ω^β, $\inf_{x\in\Gamma_D, y\in\Gamma} |x-y| \ge \kappa_0 > 0$, $\Gamma_D^\gamma = \Gamma_D \cap \overline{\Omega^\gamma}$, $\Gamma_N^\gamma = \partial\Omega^\gamma \setminus (\overline{\Gamma} \cup \overline{\Gamma_D})$, $\gamma = \alpha, \beta$;

(A2) N and N_Γ generate Young like measures $\mu = N \mathrm{d}E$ on G and $\mu_\Gamma = N_\Gamma \mathrm{d}E$ on G_Γ. $\int_{E_G} \mu(x, \mathrm{d}E) \le \widehat{c}$ a.e. in Ω, $\int_{E_G} \mu_\Gamma(x, \mathrm{d}E) \le \widehat{c}$ a.e. on Γ;

(A3) $G_{phot} \in L^\infty(\mathbb{R}_+, L_+^\infty(\Omega))$, $\|G_{phot}(t)\|_{L^\infty} \le c$ f.a.a. $t \in \mathbb{R}_+$,
$k_0 \in L_+^\infty(\Omega)$, $k_0 \ge c > 0$ a.e., $r_0 : \Omega \times \mathbb{R}_+^2 \to \mathbb{R}_+$, $r_0(x, \cdot)$ Lipschitzian, uniformly w.r.t. $x \in \Omega$, $r_0(\cdot, y)$ measurable for all $y \in \mathbb{R}_+^2$, $r_0(\cdot, 0) \in L^\infty(\Omega)$,
r_i, $k_i \in L_+^\infty(G; \mathrm{d}\mu)$, $k_i \ge c > 0$ μ-a.e. on G, $r_{\Gamma i}^\gamma$, $k_{\Gamma i}^\gamma \in L_+^\infty(G_\Gamma; \mathrm{d}\mu_\Gamma)$,
$k_{\Gamma i}^\gamma \ge c > 0$ μ_Γ-a.e. on G_Γ, $\sigma_i^\gamma \in L_+^\infty(\Gamma)$, $\gamma = \alpha, \beta$, $i = 1, 2$;

(A4) $\varepsilon \in L^\infty(\Omega)$, $\varepsilon \ge c > 0$ a.e. on Ω, $f \in L^2(\Omega)$, $z^D \in W^{1,\infty}(\Omega)$, $z^D|_{\Gamma_D} = z^D$ (cf. (1.6));

(A5) $D_i \in L^\infty(\Omega)$, $D_i \ge \epsilon > 0$ a.e. on Ω, $i = 1, 2$,
$u^D = ((u_1^{\alpha D}, u_1^{\beta D}), (u_2^{\alpha D}, u_2^{\beta D}), 0, 0, 0, 0)$, $\ln u_i^{\gamma D} \in W^{1,\infty}(\Omega^\gamma)$, with
$u_i^{\gamma D}|_{\Gamma_D^\gamma} = u_i^{\gamma D}$ (cf. (1.7)), $u_i^{\gamma D}|_\Gamma = \frac{1}{\sigma_i^\gamma}$, $\gamma = \alpha, \beta$, $i = 1, 2$,
$\widetilde{u}_i \in L^\infty(G, \mathrm{d}\mu)$, $\widetilde{u}_i \ge c > 0$, $i = 3, 4$, $u_1^D \widetilde{u}_4 = k_1 \widetilde{u}_3$ μ-a.e. in G,
$\widetilde{u}_{\Gamma i} \in L^\infty(G_\Gamma, \mathrm{d}\mu_\Gamma)$, $\widetilde{u}_{\Gamma i} \ge c > 0$, $i = 1, 2$, $u_1^{\alpha D} \widetilde{u}_{\Gamma 2} = k_{\Gamma 1}^\alpha \widetilde{u}_{\Gamma 1}$ μ_Γ-a.e. in G_Γ;

(A6) $U_i \in L^\infty_+(\Omega)$, $i=1,2$, $U_3, U_4 \in L^\infty_+(G;\mathrm{d}\mu)$, $U_3, U_4 \le 1$, $U_3+U_4 = 1$ μ-a.e. on G, $U_{\Gamma 1}$, $U_{\Gamma 2} \in L^\infty_+(G_\Gamma;\mathrm{d}\mu_\Gamma)$, $U_{\Gamma 1}$, $U_{\Gamma 2} \le 1$, $U_{\Gamma 1} + U_{\Gamma 2} = 1$ μ_Γ-a.e. on G_Γ.

2.2 Weak formulation

We use the vector $U = (U_1, \dots, U_4, U_{\Gamma 1}, U_{\Gamma_2})$ and we introduce the function spaces

$$
\begin{aligned}
&Y := L^2(\Omega)^2 \times L^2(G;\mathrm{d}\mu)^2 \times L^2(G_\Gamma;\mathrm{d}\mu_\Gamma)^2, \qquad Z := H^1_0(\Omega \cup \Gamma_N),\\
&V := L^\infty(\Omega)^2 \times L^\infty(G;\mathrm{d}\mu)^2 \times L^\infty(G_\Gamma;\mathrm{d}\mu_\Gamma)^2,\\
&X := \big\{u = (u_1, ..., u_4, u_{\Gamma 1}, u_{\Gamma 2}) \in Y\colon\ u_i = (u_i^\alpha, u_i^\beta),\ u_i^\gamma \in H^1_0(\Omega^\gamma \setminus \Gamma_N^\gamma),\ \gamma = \alpha, \beta,\ i = 1, 2\big\},
\end{aligned}
$$

and define the operators $\mathcal{A}\colon [(X + u^D) \cap V_+] \times (Z + z^D)] \to X^*$, $\mathcal{R}\colon [X + u^D] \cap V_+ \to X^*$, and $\mathcal{P}\colon (Z + z^D) \times Y \to Z^*$ by

$$
\begin{aligned}
\langle \mathcal{A}(u,z), \widehat{u}\rangle_X :=& \sum_{i=1}^2 \int_\Omega D_i(\nabla u_i + \lambda_i u_i \nabla z)\cdot\nabla \widehat{u}_i \,\mathrm{d}x, \quad \widehat{u} \in X,\\
\langle \mathcal{R}(u), \widehat{u}\rangle_X :=& \sum_{i=1}^2 \Big\{ \int_\Omega \{r_0(u_1u_2 - k_0) - G_{phot}\}\widehat{u}_i \,\mathrm{d}x + \int_\Gamma (\sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta)(\widehat{u}_i^\alpha - \widehat{u}_i^\beta)\,\mathrm{d}a\Big\}\\
&+ \int_G \Big\{ r_1(u_1u_4 - k_1u_3)(\widehat{u}_1 + \widehat{u}_4 - \widehat{u}_3) + r_2(u_2u_3 - k_2u_4)(\widehat{u}_2 + \widehat{u}_3 - \widehat{u}_4)\Big\}\,\mathrm{d}\mu\\
&+ \sum_{\gamma=\alpha,\beta} \int_{G_\Gamma} \Big\{ r^\gamma_{\Gamma 1}(u_1^\gamma u_{\Gamma 2} - k^\gamma_{\Gamma 1} u_{\Gamma 1})(\widehat{u}_1^\gamma + \widehat{u}_{\Gamma 2} - \widehat{u}_{\Gamma 1})\\
&\qquad + r^\gamma_{\Gamma 2}(u_2^\gamma u_{\Gamma 1} - k^\gamma_{\Gamma 2} u_{\Gamma 2})(\widehat{u}_2^\gamma + \widehat{u}_{\Gamma 1} - \widehat{u}_{\Gamma 2})\Big\}\,\mathrm{d}\mu_\Gamma, \quad \widehat{u} \in X,\\
\langle \mathcal{P}(z,u), \overline{z}\rangle_Z :=& \int_\Omega \Big\{ \varepsilon \nabla z \cdot \nabla \widehat{z} - \big[f + \sum_{i=1}^2 \lambda_i u_i\big]\,\widehat{z}\Big\}\,\mathrm{d}x - \sum_{i=3}^4 \int_G \lambda_i u_i \widehat{z}\,\mathrm{d}\mu\\
&- \sum_{i=1}^2 \int_{G_\Gamma} \lambda_{\Gamma i} u_{\Gamma i} \widehat{z}\,\mathrm{d}\mu_\Gamma, \quad \widehat{z} \in Z.
\end{aligned}
$$

Note that here integrals over Ω of expressions containing u_1, u_2 or ∇u_1, ∇u_2 take into account the values of u_i^γ or ∇u_i^γ on Ω^γ, $i = 1, 2$. Then the weak formulation of the electronic model for solar cells with active interfaces (1.1) – (1.8) reads as

$$
\left.\begin{aligned}
u'(t) + \mathcal{A}(u(t), z(t)) + \mathcal{R}(u(t)) = 0, \quad \mathcal{P}(z(t), u(t)) = 0, \quad \text{f.a.a. } t > 0,\\
u(0) = U, \quad u \in H^1_{\mathrm{loc}}(\mathbb{R}_+, X^*) \cap L^\infty_{\mathrm{loc}}(\mathbb{R}_+, V_+),\\
u - u^D \in L^2_{\mathrm{loc}}(\mathbb{R}_+, X), \quad z - z^D \in L^2_{\mathrm{loc}}(\mathbb{R}_+, Z) \cap L^\infty_{\mathrm{loc}}(\mathbb{R}_+, L^\infty(\Omega)).
\end{aligned}\right\} \qquad \text{(P)}
$$

3 A priori estimates

3.1 Energy estimates

To prove the thermodynamic correctness of the model we need three preparatory lemmas.

Lemma 3.1 *We assume* (A1), (A2), (A4). *For any $u \in Y$ there exists a unique solution $z \in Z + z^D$ to $\mathcal{P}(z,u) = 0$. Moreover there is a constant $c > 0$ such that*

$$\|z - \widehat{z}\|_Z \le c\,\|u - \widehat{u}\|_Y \quad \forall u, \widehat{u} \in Y,\ \mathcal{P}(z,u) = \mathcal{P}(\widehat{z},\widehat{u}) = 0. \tag{3.1}$$

Let $S = [0,T]$, $T > 0$. Then for every $u \in L^2(S,Y)$ there exists a unique $z \in L^2(S,Z) + z^D$ such that $\mathcal{P}(z(t),u(t)) = 0$ f.a.a. $t \in S$. If $u \in C(S,Y)$ then $z \in C(S,Z) + z^D$ follows and the last equation is fulfilled for all $t \in S$.

Proof. 1. The problem $\mathcal{P}(z,u) = 0$ may be written equivalently by $\mathcal{P}_0(z - z^D) = g(z^D,u)$ with $g(z^D,u)$ and the Lipschitz continuous and strongly monotone operator $\mathcal{P}_0 \colon Z \to Z^*$,

$$\langle g(z^D,u), \widehat{y}\rangle_Z = \int_\Omega \Big\{ \big(f + \sum_{i=1}^{2} \lambda_i u_i\big)\widehat{y} - \varepsilon \nabla z^D \cdot \nabla \widehat{y} \Big\} \mathrm{d}x + \sum_{i=3}^{4} \int_G \lambda_i u_i \widehat{y}\, \mathrm{d}\mu + \sum_{i=1}^{2} \int_{G_\Gamma} \lambda_{\Gamma i} u_{\Gamma i} \widehat{y}\, \mathrm{d}\mu_\Gamma,$$

$$\langle \mathcal{P}_0 y, \widehat{y}\rangle_Z = \int_\Omega \varepsilon \nabla y \cdot \nabla \widehat{y}\, \mathrm{d}x, \quad y,\, \widehat{y} \in Z.$$

To show $g(z^D,u) \in Z^*$, for the last two terms we argue as follows: Because of (A2) we have

$$\int_G u_{i+2} \widehat{y}\, \mathrm{d}\mu \le c\|u_{i+2}\|_{L^2(G;\mathrm{d}\mu)} \|\widehat{y}\|_Z, \ \int_{G_\Gamma} u_{\Gamma i} \widehat{y}\, \mathrm{d}\mu_\Gamma \le c\|u_{\Gamma i}\|_{L^2(G_\Gamma;\mathrm{d}\mu_\Gamma)} \|\widehat{y}\|_Z,\ \widehat{y} \in Z,\ i = 1,2.$$

Therefore, for all right-hand sides $g(z^D,u) \in Z^*$ there is a unique solution to $\mathcal{P}_0(z - z^D) = g(z^D,u)$ and (3.1) follows immediately. As a direct consequence we obtain the result for the time dependent functions. ☐

Remark 3.1 *If (u,z) is a solution to* (P) *then $u \in C(\mathbb{R}_+,Y)$. Thus, by Lemma 3.1 $z - z^D \in C(\mathbb{R}_+,Z)$ and for all $t \in \mathbb{R}_+$ the relations $\mathcal{P}(z(t),u(t)) = 0$ in Z^*, $u_i(t) \ge 0$ a.e. on Ω, $i = 1,2$, $u_i(t) \ge 0$ μ-a.e. on G, $i = 3,4$, $u_{\Gamma i}(t) \ge 0$, μ_Γ-a.e. on G_Γ, $i = 1,2$, are fulfilled.*

Lemma 3.2 i) *We assume* (A1) – (A6). *If (u,z) is a solution to* (P) *then for all $t \in \mathbb{R}_+$*

$$u_3(t) + u_4(t) = U_3 + U_4 = 1, \quad 0 \le u_3(t),\, u_4(t) \le 1 \quad \mu\text{-a.e. on } G,$$
$$u_{\Gamma 1}(t) + u_{\Gamma 2}(t) = U_{\Gamma 1} + U_{\Gamma 2} = 1, \quad 0 \le u_{\Gamma 1}(t),\, u_{\Gamma 2}(t) \le 1 \quad \mu_\Gamma\text{-a.e. on } G_\Gamma.$$

ii) *We assume* (A1) – (A6). *Then there exist constants $q > 2$ and $c > 0$ such that*

$$\|z\|_{W^{1,q}} \le c\Big\{1 + \sum_{i=1}^{2} \|u_i\|_{L^{2q/(2+q)}}\Big\} \tag{3.2}$$

for any solution (u,z) to (P).

Proof. i) The result for u_3 and u_4 is obtained as in the proof of [9, Lemma 3.2]. By similar ideas, now testing the ODEs for $u_{\Gamma 1}$ and $u_{\Gamma 2}$ by $\mu_\Gamma(B_\varrho^{G_\Gamma}(y))^{-1}\chi_{B_\varrho^{G_\Gamma}(y)}$ (where $B_\varrho^{G_\Gamma}(y)$ is the intersection of G_Γ and the ball centered at y with radius ϱ and χ denotes the characteristic function) and letting $\varrho\downarrow 0$ the assertions for $u_{\Gamma 1}$ and $u_{\Gamma 2}$ follow.

ii) We use the notation of the proof of Lemma 3.1. According to Gröger's regularity result for elliptic equations with nonsmooth data [13, Theorem 1] and (A4), (A1) we can fix a $q = q(\Omega,\varepsilon) > 2$ such that, if

$$\forall \widehat{y}\in H_0^1(\Omega\cup\Gamma_N):\ \langle\mathcal{P}_0 y,\widehat{y}\rangle_Z = \langle g,\widehat{y}\rangle,\quad g\in W^{-1,q}(\Omega\cup\Gamma_N),\, y\in H_0^1(\Omega\cup\Gamma_N)$$

then $y\in W_0^{1,q}(\Omega\cup\Gamma_N)$. We set

$$r=\frac{2q}{q-2},\quad r'=\frac{2q}{q+2},\quad s=\frac{q}{q-2},\quad s'=\frac{q}{2}. \tag{3.3}$$

Note that $g(z^D,u)\in W^{-1,q}(\Omega\cup\Gamma_N)$. We use again (A2) to estimate

$$\int_G u_{i+2}\widehat{y}\,\mathrm{d}\mu \le c\|u_{i+2}\|_{L^{r'}(G;\mathrm{d}\mu)}\|\widehat{y}\|_{L^r} \le c\|u_{i+2}\|_{L^{r'}(G;\mathrm{d}\mu)}\|\widehat{y}\|_{W^{1,q'}},$$

$$\int_{G_\Gamma} u_{\Gamma i}\widehat{y}\,\mathrm{d}\mu_\Gamma \le c\|u_{\Gamma i}\|_{L^{s'}(G_\Gamma;\mathrm{d}\mu_\Gamma)}\|\widehat{y}\|_{L^s(\Gamma)} \le c\|u_{\Gamma i}\|_{L^{s'}(G_\Gamma;\mathrm{d}\mu_\Gamma)}\|\widehat{y}\|_{W^{1,q'}},\quad i=1,2.$$

Gröger's regularity result thus implies

$$\|z-z^D\|_{W_0^{1,q}}\le c\|g(z^D,u)\|_{W^{-1,q}}\le c\Big(1+\sum_{i=1}^2\|u_i\|_{L^{r'}}+\sum_{i=3}^4\|u_i\|_{L^{r'}(G;\mathrm{d}\mu)}+\sum_{i=1}^2\|u_{\Gamma i}\|_{L^{s'}(G_\Gamma;\mathrm{d}\mu_\Gamma)}\Big).$$

Therefore, due to (A4) and part i) of Lemma 3.2 the desired estimate follows. □

Lemma 3.3 *We assume* (A1) – (A6). *Then for all* $\tau>0$ *there exist constants* $c_\tau>0$, $c>0$ *such that*

$$\int_0^t\Big\{\sum_{\gamma=\alpha,\beta}\big(\|r_{\Gamma 1}^\gamma u_1^\gamma u_{\Gamma 2}\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)}+\|r_{\Gamma 2}^\gamma u_2^\gamma u_{\Gamma 1}\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)}\big)+\sum_{i=1}^2\Big|\int_\Gamma \sigma_i^\alpha u_i^\alpha-\sigma_i^\beta u_i^\beta\,\mathrm{d}a\Big|\Big\}\mathrm{d}s$$

$$\le c+\int_0^t\Big\{c+\sum_{i=1}^2\big\{\tau\|2\nabla\sqrt{u_i}+\lambda_i\sqrt{u_i}\,\nabla z\|_{L^2(\Omega)}^2+c_\tau\|u_i\|_{L^1(\Omega)}\big\}\Big\}\mathrm{d}s\quad \forall t>0$$

for any solution (u,z) *to* (P).

Proof. Due to (A1), for $\gamma=\alpha,\beta$ we find Lipschitz continuous functions $\phi^\gamma:\overline{\Omega^\gamma}\to[0,1]$ with $\phi^\gamma=0$ on Γ_D^γ, $\phi^\gamma=1$ on Γ and $|\nabla\phi^\gamma|\le 1/\kappa_0$. Testing the equations for u_i, $i=1,2$, on Ω^α by ϕ^α, adding them and having in mind Lemma 3.2 i), (A4), (A5), (A6) we obtain

$$\sum_{i=1}^2\|u_i(t)\phi^\alpha\|_{L^1(\Omega^\alpha)}+\int_0^t\Big\{\int_{\Omega^\alpha}2r_0u_1u_2\phi^\alpha\,\mathrm{d}x+\int_{\Omega^\alpha\times E_G}(r_1u_1u_4+r_2u_2u_3)\phi^\alpha\mathrm{d}\mu\Big\}\mathrm{d}s$$

$$+\int_0^t\Big\{\int_{G_\Gamma}(r_{\Gamma 1}^\alpha u_1^\alpha u_{\Gamma 2}+r_{\Gamma 2}^\alpha u_2^\alpha u_{\Gamma 1})\,\mathrm{d}\mu_\Gamma+\sum_{i=1}^2\int_\Gamma(\sigma_i^\alpha u_i^\alpha-\sigma_i^\beta u_i^\beta)\,\mathrm{d}a\Big\}\mathrm{d}s$$

$$\le\sum_{i=1}^2\Big\{\|U_i\|_{L^1(\Omega^\alpha)}+\int_0^t\Big\{c+\int_{\Omega^\alpha}\frac{D_i}{\kappa_0}|\nabla u_i+\lambda_iu_i\nabla z|\mathrm{d}x\Big\}\mathrm{d}s\Big\}\quad\forall t>0.$$

The terms in the first line can be left out since they are nonnegative. The last term in the last line can be estimated as follows where at the end Young's inequality is used

$$\int_{\Omega^\alpha} \frac{D_i}{\kappa_0} |\nabla u_i + \lambda_i u_i \nabla z| \,\mathrm{d}x \le c \int_{\Omega^\alpha} \sqrt{u_i} |2\nabla\sqrt{u_i} + \lambda_i \sqrt{u_i}\, \nabla z| \,\mathrm{d}x$$
$$\le \tau \|2\nabla\sqrt{u_i} + \lambda_i\sqrt{u_i}\,\nabla z\|^2_{L^2(\Omega^\alpha)} + c_\tau \|u_i\|_{L^1(\Omega^\alpha)}.$$

Similar results are obtained by testing the equations for u_i, $i=1,2$, on Ω^β by ϕ^β, only the term $\int_\Gamma (\sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta)\,\mathrm{d}a$ then has the opposite sign. Combining both estimates, the assertion of the lemma follows. □

Using z^D, $u_1^{\gamma D}$, $u_2^{\gamma D}$ and $\widetilde{u}_3$, $\widetilde{u}_4$, $\widetilde{u}_{\Gamma 1}$, $\widetilde{u}_{\Gamma 2}$ from (A5), we define functionals $\widetilde{F}_1$, $\widetilde{F}_2 \colon Y_+ \to \mathbb{R}$,

$$\widetilde{F}_1(u) := \int_\Omega \frac{\varepsilon}{2} |\nabla(z - z^D)|^2 \,\mathrm{d}x,$$
$$\widetilde{F}_2(u) := \int_\Omega \sum_{i=1}^{2} \big\{ u_i (\ln \frac{u_i}{u_i^D} - 1) + u_i^D \big\} \,\mathrm{d}x + \sum_{i=3}^{4} \int_G \big\{ u_i \ln \frac{u_i}{\widetilde{u}_i} - u_i + \widetilde{u}_i \big\} \,\mathrm{d}\mu$$
$$+ \sum_{i=1}^{2} \int_{G_\Gamma} \big\{ u_{\Gamma i} \ln \frac{u_{\Gamma i}}{\widetilde{u}_{\Gamma i}} - u_{\Gamma i} + \widetilde{u}_{\Gamma i} \big\} \,\mathrm{d}\mu_\Gamma,$$

where z is the solution to $\mathcal{P}(z,u) = 0$ (see Lemma 3.1). The value $\widetilde{F}_1(u) + \widetilde{F}_2(u)$ can be interpreted as free energy of the state u. Because of (A4) we find for $u \in Y_+$ the estimate

$$\widetilde{F}_1(u) + \widetilde{F}_2(u)$$
$$\ge c\Big(\|z - z^D\|_Z^2 + \sum_{i=1}^{2} \|u_i \ln u_i\|_{L^1} + \sum_{i=3}^{4} \|u_i \ln u_i\|_{L^1(G,\mathrm{d}\mu)} + \sum_{i=1}^{2} \|u_{\Gamma i} \ln u_{\Gamma i}\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)} \Big) - \widetilde{c}.$$

We extend $\widetilde{F}_k$, $k=1,2$, to arguments from the space X^* by the definition

$$F_k := (\widetilde{F}_k^*|_X)^* \colon X^* \to \overline{\mathbb{R}}, \quad k = 1,2.$$

The star denotes the conjugation (see [3]). Following the ideas in [9, Subsection 3.4] we find that the free energy functional $F := F_1 + F_2$ is proper, convex and lower semicontinuous. For $u \in Y_+$ the relation $F(u) = \widetilde{F}_1(u) + \widetilde{F}_2(u)$ is fulfilled, $F|_{Y_+}$ is continuous. Moreover, if $u \in Y_+$, $u > \delta$ and $(\ln \frac{u_1}{u_1^D}, \ln \frac{u_2}{u_2^D}, \ln \frac{u_3}{\widetilde{u}_3}, \ln \frac{u_4}{\widetilde{u}_4}, \ln \frac{u_{\Gamma 1}}{\widetilde{u}_{\Gamma 1}}, \ln \frac{u_{\Gamma 2}}{\widetilde{u}_{\Gamma 2}}) \in X$, then

$$\lambda(z - z^D) + \big(\ln \frac{u_1}{u_1^D}, \ln \frac{u_2}{u_2^D}, \ln \frac{u_3}{\widetilde{u}_3}, \ln \frac{u_4}{\widetilde{u}_4}, \ln \frac{u_{\Gamma 1}}{\widetilde{u}_{\Gamma 1}}, \ln \frac{u_{\Gamma 2}}{\widetilde{u}_{\Gamma 2}} \big) \in \partial F(u).$$

Theorem 3.1 *We assume* (A1)–(A6). *Let* (u,z) *be a solution to* (P) *and* $T \in \mathbb{R}_+$. *Then*

$$F(u(t)) \le (F(U) + c_0) e^{c_0 t} \quad \forall t \in [0,T],$$

where $c_0 > 0$ *is a constant independent of* U *and* T. *Moreover, if*

$$G_{phot} = 0,\ u_1^D u_2^D = k_0,\ \ln u_i^{\gamma D} + \lambda_i z^D \text{ is constant on } \Omega^\gamma,\ \gamma = \alpha,\beta,\ i = 1,2, \tag{3.4}$$

and if

$$k_1 k_2 = u_1^D u_2^D \ \mu\text{-a.e. on } G,\ \frac{k_{\Gamma 1}^\alpha}{k_{\Gamma 1}^\beta} = \frac{u_1^{\alpha D}}{u_1^{\beta D}},\ k_{\Gamma 1}^\gamma k_{\Gamma 2}^\gamma = u_1^{\gamma D} u_2^{\gamma D},\ \mu_\Gamma\text{-a.e. on } G_\Gamma, \tag{3.5}$$

$\gamma = \alpha, \beta$, *then* c_0 *can be chosen as zero.*

Proof. 1. We use formally the test function

$$\lambda(z-z^D)+\big(\ln\frac{u_1}{u_1^D},\ln\frac{u_2}{u_2^D},\ln\frac{u_3}{\widetilde{u}_3},\ln\frac{u_4}{\widetilde{u}_4},\ln\frac{u_{\Gamma1}}{\widetilde{u}_{\Gamma1}},\ln\frac{u_{\Gamma2}}{\widetilde{u}_{\Gamma2}}\big)$$

for (P) and apply Brézis formula (see Lemma 6.1 or [2, Lemma 3.3]). (To derive the desired result precisely, one has to use test functions

$$\lambda(z-z^D)+\big(\ln\frac{u_1^\delta}{u_1^D},\ln\frac{u_2^\delta}{u_2^D},\ln\frac{u_3^\delta}{\widetilde{u}_3},\ln\frac{u_4^\delta}{\widetilde{u}_4},\ln\frac{u_{\Gamma1}^\delta}{\widetilde{u}_{\Gamma1}},\ln\frac{u_{\Gamma2}^\delta}{\widetilde{u}_{\Gamma2}}\big),\quad u^\delta=\max\{u,\delta\},$$

$$0<\delta<\min\big\{\min_{i=1,2}\{\operatorname*{ess\,inf}_\Omega U_i,\operatorname*{ess\,inf}_\Omega u_i^D\},\min_{i=3,4}\{\operatorname*{ess\,inf}_{G,\mu} U_i\},\min_{i=1,2}\{\operatorname*{ess\,inf}_{G_\Gamma,\mu_\Gamma} U_{\Gamma i}\}\big\},\tag{3.6}$$

and then one has to take the limit $\delta\downarrow 0$, see steps $1,2$ in the proof of [9, Theorem 3.2].)

2. We estimate a.e. in Ω

$$D_i(\nabla u_i+\lambda_i u_i\nabla z)\cdot\nabla(\ln\tfrac{u_i}{u_i^D}+\lambda_i(z-z^D))\ge\frac{\epsilon}{2}|2\nabla\sqrt{u_i}+\lambda_i\sqrt{u_i}\nabla z|^2-cu_i|\nabla(\ln u_i^D+\lambda_i z^D)|^2,$$
$$G_{phot}(\ln\tfrac{u_i}{u_i^D}+\lambda_i(z-z^D))\le|G_{phot}|(|u_i|+|\ln u_i^D|+|z-z^D|),$$
$$r_0(u_1u_2-k_0)\ln\tfrac{u_1u_2}{u_1^Du_2^D}\ge-c|\ln\tfrac{u_1^Du_2^D}{k_0}|.$$

The last line follows by a case by case analysis. Have in mind that all considered reactions are charge conserving. Moreover, we find by the monotonicity of the logarithm function and by $u_1^D\widetilde{u}_4=k_1\widetilde{u}_3$ (see (A5)) that μ-a.e. on G

$$r_1(u_1u_4-k_1u_3)\ln\tfrac{u_1u_4\widetilde{u}_3}{u_1^D\widetilde{u}_4u_3}=r_1(u_1u_4-k_1u_3)\ln\tfrac{u_1u_4}{k_1u_3}\ge0,$$
$$r_2(u_2u_3-k_2u_4)\ln\tfrac{u_2u_3\widetilde{u}_4}{u_2^D\widetilde{u}_3u_4}=r_2(u_2u_3-k_2u_4)\Big[\ln\tfrac{u_2u_3}{k_2u_4}+\ln\tfrac{k_1k_2}{u_1^Du_2^D}\Big]\ge-c(|u_2|+1)|\ln\tfrac{k_1k_2}{u_1^Du_2^D}|.$$

Additionally, using that $u_1^{\alpha D}\widetilde{u}_{\Gamma2}=k_{\gamma1}^\alpha\widetilde{u}_{\Gamma1}$ (see (A5)) we establish that μ_Γ-a.e. on G_Γ

$$\begin{aligned}
r_{\Gamma1}^\alpha(u_1^\alpha u_{\Gamma2}-k_{\Gamma1}^\alpha u_{\Gamma1})\ln\tfrac{u_1^\alpha u_{\Gamma2}\widetilde{u}_{\Gamma1}}{u_1^{\alpha D}\widetilde{u}_{\Gamma2}u_{\Gamma1}}&=r_{\Gamma1}^\alpha(u_1^\alpha u_{\Gamma2}-k_{\Gamma1}^\alpha u_{\Gamma1})\ln\tfrac{u_1^\alpha u_{\Gamma2}}{k_{\Gamma1}^\alpha u_{\Gamma1}}\ge0,\\
r_{\Gamma1}^\beta(u_1^\beta u_{\Gamma2}-k_{\Gamma1}^\beta u_{\Gamma1})\ln\tfrac{u_1^\beta u_{\Gamma2}\widetilde{u}_{\Gamma1}}{u_1^{\beta D}\widetilde{u}_{\Gamma2}u_{\Gamma1}}&=r_{\Gamma1}^\beta(u_1^\beta u_{\Gamma2}-k_{\Gamma1}^\beta u_{\Gamma1})\Big[\ln\tfrac{u_1^\beta u_{\Gamma2}}{k_{\Gamma1}^\beta u_{\Gamma1}}+\ln\tfrac{k_{\Gamma1}^\beta u_1^{\alpha D}}{k_{\Gamma1}^\alpha u_1^{\beta D}}\Big]\\
&\ge-(r_{\Gamma1}^\beta u_1^\beta u_{\Gamma2}+c)|\ln\tfrac{k_{\Gamma1}^\beta u_1^{\alpha D}}{k_{\Gamma1}^\alpha u_1^{\beta D}}|,\\
r_{\Gamma2}^\alpha(u_2^\alpha u_{\Gamma1}-k_{\Gamma2}^\alpha u_{\Gamma2})\ln\tfrac{u_2^\alpha u_{\Gamma1}\widetilde{u}_{\Gamma2}}{u_2^{\alpha D}\widetilde{u}_{\Gamma1}u_{\Gamma2}}&=r_{\Gamma2}^\alpha(u_2^\alpha u_{\Gamma1}-k_{\Gamma2}^\alpha u_{\Gamma2})\Big[\ln\tfrac{u_2^\alpha u_{\Gamma1}}{k_{\Gamma2}^\alpha u_{\Gamma2}}+\ln\tfrac{k_{\Gamma1}^\alpha k_{\Gamma2}^\alpha}{u_1^{\alpha D}u_2^{\alpha D}}\Big]\\
&\ge-(r_{\Gamma2}^\alpha u_2^\alpha u_{\Gamma1}+c)|\ln\tfrac{k_{\Gamma1}^\alpha k_{\Gamma2}^\alpha}{u_1^{\alpha D}u_2^{\alpha D}}|,\\
r_{\Gamma2}^\beta(u_2^\beta u_{\Gamma1}-k_{\Gamma2}^\beta u_{\Gamma2})\ln\tfrac{u_2^\beta u_{\Gamma1}\widetilde{u}_{\Gamma2}}{u_2^{\beta D}\widetilde{u}_{\Gamma1}u_{\Gamma2}}&=r_{\Gamma2}^\beta(u_2^\beta u_{\Gamma1}-k_{\Gamma2}^\beta u_{\Gamma2})\Big[\ln\tfrac{u_2^\beta u_{\Gamma1}}{k_{\Gamma2}^\beta u_{\Gamma2}}+\ln\tfrac{k_{\Gamma1}^\alpha k_{\Gamma2}^\beta}{u_1^{\alpha D}u_2^{\beta D}}\Big]\\
&\ge-(r_{\Gamma2}^\beta u_2^\beta u_{\Gamma1}+c)|\ln\tfrac{k_{\Gamma1}^\alpha k_{\Gamma2}^\beta}{u_1^{\alpha D}u_2^{\beta D}}|,
\end{aligned}$$

and by $u_i^{\gamma D}|_\Gamma=\frac{1}{\sigma_i^\gamma}$ $i=1,2$, $\gamma=\alpha,\beta$, (see (A5)) we conclude that

$$(\sigma_i^\alpha u_i^\alpha-\sigma_i^\beta u_i^\beta)\ln\tfrac{u_i^\alpha u_i^{\beta D}}{u_i^{\alpha D}u_i^\beta}=(\sigma_i^\alpha u_i^\alpha-\sigma_i^\beta u_i^\beta)\ln\tfrac{\sigma_i^\alpha u_i^\alpha}{\sigma_i^\beta u_i^\beta}=0\qquad\text{a.e. on }\Gamma,\quad i=1,2.$$

According to our assumptions (A3), (A4) and (A5) we find from step 1 and the previous estimates

$$
\begin{aligned}
&F(u(t)) - F(U) + \frac{\epsilon}{2}\int_0^t \|2\nabla\sqrt{u_i} + \lambda_i\sqrt{u_i}\,\nabla z\|_{L^2}^2\,\mathrm{d}s\\
&\le c\int_0^t \sum_{i=1}^2 (1+\|u_i\|_{L^1})\Big(\|\nabla(\ln u_i^D + \lambda_i z^D)\|_{L^\infty}^2 + \|\ln \tfrac{u_1^D u_2^D}{k_0}\|_{L^\infty} + \|\ln \tfrac{k_1k_2}{u_1^D u_2^D}\|_{L^\infty(G,\mathrm{d}\mu)}\Big)\mathrm{d}s\\
&\quad + c\int_0^t (1 + \|r_{\Gamma 1}^\beta u_1^\beta u_{\Gamma 2}\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)})\|\ln \tfrac{k_{\Gamma 1}^\beta u_1^{\alpha D}}{k_{\Gamma 1}^\alpha u_1^{\beta D}}\|_{L^\infty(G_\Gamma,\mathrm{d}\mu_\Gamma)}\,\mathrm{d}s\\
&\quad + c\int_0^t (1 + \|r_{\Gamma 2}^\alpha u_2^\alpha u_{\Gamma 1}\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)})\|\ln \tfrac{k_{\Gamma 1}^\alpha k_{\Gamma 2}^\alpha}{u_1^{\alpha D} u_2^{\alpha D}}\|_{L^\infty(G_\Gamma,\mathrm{d}\mu_\Gamma)}\,\mathrm{d}s\\
&\quad + c\int_0^t (1 + \|r_{\Gamma 2}^\beta u_2^\beta u_{\Gamma 1}\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)})\|\ln \tfrac{k_{\Gamma 1}^\alpha k_{\Gamma 2}^\beta}{u_1^{\alpha D} u_2^{\beta D}}\|_{L^\infty(G_\Gamma,\mathrm{d}\mu_\Gamma)}\,\mathrm{d}s\\
&\quad + \int_0^t \|G_{phot}\|_{L^\infty}\Big\{\sum_{i=1}^2 \big(\|u_i\|_{L^1} + \|\ln u_i^D\|_{L^1}\big) + \|z - z^D\|_{L^1}\Big\}\,\mathrm{d}s.
\end{aligned}
$$

3. If (3.4) and (3.5) are fulfilled, then the right-hand side of the previous estimate is zero. Therefore the last assertion of the theorem follows immediately. For the more general situation we argue as follows: Using (A3), (A4), (A5) and Lemma 3.3 the right hand side in the previous estimate can be majorized by

$$
\int_0^t \sum_{i=1}^2 \Big(c\big(\|u_i\|_{L^1} + \|z - z^D\|_Z^2 + 1\big) + \frac{\epsilon}{2}\|2\nabla\sqrt{u_i} + \lambda_i\sqrt{u_i}\,\nabla z\|_{L^2}^2\Big)\,\mathrm{d}s.
$$

Since $\sum_{i=1}^2 \|u_i\|_{L^1} + \|z - z^D\|_Z^2 \le cF(u) + c$ for z with $\mathcal{P}(z,u) = 0$, Gronwall's lemma supplies the desired result. $\square$

Remark 3.2 *Theorem 3.1 guarantees that the electronic model for solar cells including interface kinetics and energy resolved defect densities in Ω and at the interface Γ is thermodynamically correct. The free energy functional F is something like a Lyapunov function. Namely, under the special assumptions* (3.4) *and* (3.5) (*meaning that the data is compatible with thermodynamic equilibrium*) *the function $t \mapsto F(u(t))$ is monotonously decreasing. For the more general case of data the free energy may be increasing, but its growth can be estimated by Theorem 3.1.*

Remark 3.3 *If r_0 is independent of u_1, u_2 and G_{phot} is independent of time, and the Dirichlet values and reaction constants fulfill*

$$
u_1^D u_2^D = k_0 + \frac{G_{phot}}{r_0},\ \ln u_i^{\gamma D} + \lambda_i z^D \text{ is constant on } \Omega^\gamma,\ \gamma = \alpha, \beta,\ i = 1, 2, \tag{3.7}
$$

instead of (3.4) *in Theorem 3.1 and if additionally* (3.5) *holds true, then the free energy on solutions $F(u(t))$ decreases monotonously, too. This can be seen by substituting the second and third estimate in step 2 of the proof of Theorem 3.1 by*

$$
r_0\Big(u_1u_2 - k_0 - \frac{G_{phot}}{r_0}\Big)\ln\frac{u_1u_2}{u_1^D u_2^D} \ge -\Big|\ln\frac{u_1^D u_2^D}{k_0 + \frac{G_{phot}}{r_0}}\Big|,
$$

which is obtained by a case by case analysis, too.

3.2 L^∞-estimates of the solution

Have in mind that Lemma 3.2 provides global upper and lower bounds for u_3, u_4 on G and $u_{\Gamma 1}$, $u_{\Gamma 2}$ on G_Γ. To prove upper bounds for the densities of electrons and holes we argue in two steps. Starting with estimates of the $L^\infty(\mathbb{R}_+, L^2)$-norm of u_i, $i=1,2$, (see Lemma 3.4), the final estimate is obtained by Moser iteration in Theorem 3.2.

Lemma 3.4 *Under the assumptions* (A1) – (A6) *there exists a monotonous function* $d : \mathbb{R}_+ \to \mathbb{R}_+$ *depending only on the data* (*but not on* T) *such that*

$$\sum_{i=1}^{2} \|u_i(t)\|_{L^2} \le d(\|F(u)\|_{C(S)}) \quad \forall t \in S = [0,T]$$

for any solution (u,z) *to* (P).

Proof. For problem (P) we use the test function $\mathrm{e}^{2t}(v_1, v_2, 0, \dots, 0)$,

$$v_i := (u_i - K)^+, \quad \text{where } K \ge \widehat{K} := \max\big(1, \|U\|_V, \max_{i=1,2,\ \gamma=\alpha,\beta} \|u_i^{\gamma D}\|_{L^\infty(\Omega^\gamma)}\big) \tag{3.8}$$

will be fixed later. The choice of $\widehat{K}$ ensures that $v_i^\gamma(0) = 0$, $v_i^\gamma|_{\Gamma_D^\gamma} = 0$, $\gamma = \alpha, \beta$, $i = 1,2$.

$$\begin{aligned}
&\frac{\mathrm{e}^{2t}}{2} \sum_{i=1}^{2} \int_\Omega v_i(t)^2 \,\mathrm{d}x \\
&= \int_0^t \mathrm{e}^{2s} \Big\{ \int_\Omega \sum_{i=1}^{2} \big\{ v_i^2 - D_i(\nabla v_i + \lambda_i u_i \nabla z) \cdot \nabla v_i + G_{phot} v_i + r_0(\cdot, u_1, u_2)(k_0 - u_1 u_2) v_i \big\} \,\mathrm{d}x \\
&\quad + \sum_{i=1}^{2} \int_\Gamma (\sigma_i^\alpha u_i^\alpha - \sigma_i^\beta u_i^\beta)(v_i^\beta - v_i^\alpha) \,\mathrm{d}a + \int_G \big\{ r_1(k_1 u_3 - u_1 u_4) v_1 + r_2(k_2 u_4 - u_2 u_3) v_2 \big\} \,\mathrm{d}\mu \\
&\quad + \sum_{\gamma=\alpha,\beta} \int_{G_\Gamma} \big\{ r_{\Gamma 1}^\gamma (k_{\Gamma 1}^\gamma u_{\Gamma 1} - u_1^\gamma u_{\Gamma 2}) v_1^\gamma + r_{\Gamma 2}^\gamma (k_{\Gamma 2}^\gamma u_{\Gamma 2} - u_2^\gamma u_{\Gamma 1}) v_2^\gamma \big\} \,\mathrm{d}\mu_\Gamma \Big\} \mathrm{d}s \\
&\le \int_0^t \mathrm{e}^{2s} \sum_{i=1}^{2} \big\{ -\epsilon \|v_i\|_{H^1}^2 + c\|u_i\|_{L^r} \|\nabla z\|_{L^q} \|v_i\|_{H^1} + c\|v_i\|_{L^2}^2 + c \sum_{\gamma=\alpha,\beta} \|v_i^\gamma\|_{L^2(\Gamma)}^2 + cK^2 \big\} \,\mathrm{d}s.
\end{aligned}$$

The exponents $q > 2$ and r are taken from Lemma 3.2 ii) and (3.3). For the treatment of the reaction terms we refer to (A3) and Lemma 3.2 i). Moreover, due to (A2) we have $\|v_i\|_{L^2(G,\mathrm{d}\mu)} \le c\|v_i\|_{L^2(\Omega)}$, $\|v_i^\gamma\|_{L^2(G_\Gamma, \mathrm{d}\mu_\Gamma)} \le c\|v_i^\gamma\|_{L^2(\Gamma)}$, $i=1,2$. Now we apply the trace inequality (6.1), the estimate (3.2) and the three variants of the Gagliardo-Nirenberg inequality (6.2)

$$\|v_i\|_{L^2}^2 \le c\|v_i\|_{L^1} \|v_i\|_{H^1}, \qquad \|v_i\|_{L^r} \le c\|v_i\|_{L^1}^{1/r} \|v_i\|_{H^1}^{1/r'}, \qquad \|v_i\|_{L^{r'}} \le c\|v_i\|_{L^1}^{1/r'} \|v_i\|_{H^1}^{1/r},$$

with r and r' from (3.3). At the end, Young's inequality gives for all $t \in S$

$$\frac{e^{2t}}{2} \sum_{i=1}^{2} \|v_i(t)\|_{L^2}^2 \le \int_0^t \mathrm{e}^{2s} \sum_{i=1}^{2} \Big\{ \big(\widetilde{c} \sum_{j=1}^{2} \|v_j\|_{L^1} - \frac{\epsilon}{2}\big) \|v_i\|_{H^1}^2 + c(K)\big(\|v_i\|_{L^1}^2 + 1\big) \Big\} \,\mathrm{d}s \tag{3.9}$$

with a monotonously increasing function $c(K)$. For K with $\ln K > \max_{i=1,2} \|\ln u_i^D\|_{L^\infty} + 1$ we estimate

$$F(u) \geq \sum_{i=1}^{2} \int_\Omega \{u_i(\ln \tfrac{u_i}{u_i^D} - 1) + u_i^D\} \,\mathrm{d}x \geq \sum_{i=1}^{2} \int_{\{x: v_i > 0\}} u_i(\ln K - \max_{k=1,2} \|\ln u_k^D\|_{L^\infty} - 1) \,\mathrm{d}x$$
$$\geq (\ln K - \max_{k=1,2} \|\ln u_k^D\|_{L^\infty} - 1) \sum_{i=1}^{2} \|v_i\|_{L^1}.$$

Now we fix $K \geq \widehat{K}$ as a monotonously increasing function of $\|F(u)\|_{C(S)}$ fulfilling

$$\widetilde{c} \sum_{i=1}^{2} \|v_i\|_{L^1} \leq \quad \frac{\widetilde{c}\|F(u)\|_{C(S)}}{\ln K - \max_{k=1,2} \|\ln u_k^D\|_{L^\infty} - 1} < \frac{\epsilon}{2}$$

(compare Theorem 3.1); then the term in front of the H^1-norm in (3.9) is negative. It results

$$\mathrm{e}^{2t} \sum_{i=1}^{2} \|v_i(t)\|_{L^2}^2 \leq \mathrm{e}^{2t}\, c\, c(K)(\|F(u)\|_{C(S)}^2 + 1).$$

Since $u_i \leq v_i + K$ this proves the lemma. $\square$

Lemma 3.2 and Lemma 3.4, guarantee that for solutions (u, z) to (P) for all $t \in S$ the norm $\|z(t)\|_{W^{1,q}(\Omega)}$ is bounded by a continuous function of $\|F(u)\|_{C(S)}$ depending on the data but not on T. The exponent $q > 2$ is results from Lemma 3.2 ii). We write shortly

$$\kappa = \Big(\|\nabla z\|_{L^\infty(S, L^q(\Omega))} + 1\Big)^{2r}. \tag{3.10}$$

Now we establish the upper bounds for the densities of electrons and holes. The proof is based on Moser iteration techniques. Such techniques e.g. are used in [10] for problems from semiconductor technology, in [6] for the classical van Roosbroeck system and in [8] for spin-polarized drift-diffusion systems.

Theorem 3.2 *Let* (A1) – (A6) *be satisfied. Then there exists a constant $c > 0$ and a continuous function d of $\|F(u)\|_{C(S)}$ depending only on the data (but not on T) such that*

$$\sum_{i=1}^{2} \|u_i(t)\|_{L^\infty} \leq c\,\kappa \sum_{i=1}^{2} \Big(\sup_{s \in S} \|u_i(s)\|_{L^1} + 1\Big), \quad \|z(t)\|_{L^\infty} \leq d(\|F(u)\|_{C(S)}) \quad \forall t \in S$$

for any solution (u, z) to (P).

Note that $\sup_{s \in S} \|u_i(s)\|_{L^1} \leq c\,(\|F(u)\|_{C(S)} + 1)$, $i = 1, 2$, on solutions to (P) and that this right hand side is bounded by Theorem 3.1.

Proof. Using for (P) the test functions

$$p\,\mathrm{e}^{pt}\,(v_1^{p-1}, v_2^{p-1}, 0, \ldots, 0) \in L^2(S, X),\ p = 2^m,\ m \geq 1,\ \text{where } v_i := (u_i - \widehat{K})^+,\ i = 1, 2,$$

with $\widehat{K}$ from (3.8) we obtain

$$
\begin{aligned}
&\mathrm{e}^{pt}\sum_{i=1}^{2}\int_\Omega v_i(t)^p\,\mathrm{d}x\\
&=\int_0^t p\mathrm{e}^{2s}\Big\{\int_\Omega\sum_{i=1}^{2}\big\{v_i^p-D_i(\nabla v_i+\lambda_i u_i\nabla z)\cdot\nabla v_i^{p-1}+G_{phot}v_i^{p-1}+r_0(k_0-u_1u_2)v_i^{p-1}\big\}\,\mathrm{d}x\\
&\quad+\sum_{i=1}^{2}\int_\Gamma(\sigma_i^\alpha u_i^\alpha-\sigma_i^\beta u_i^\beta)\big((v_i^\beta)^{p-1}-(v_i^\alpha)^{p-1}\big)\,\mathrm{d}a\\
&\quad+\int_G\big\{r_1(k_1u_3-u_1u_4)v_1^{p-1}+r_2(k_2u_4-u_2u_3)v_2^{p-1}\big\}\,\mathrm{d}\mu\\
&\quad+\sum_{\gamma=\alpha,\beta}\int_{G_\Gamma}\big\{r_{\Gamma1}^\gamma(k_{\Gamma1}^\gamma u_{\Gamma1}-u_1^\gamma u_{\Gamma2})(v_1^\gamma)^{p-1}+r_{\Gamma2}^\gamma(k_{\Gamma2}^\gamma u_{\Gamma2}-u_2^\gamma u_{\Gamma1})(v_2^\gamma)^{p-1}\big\}\,\mathrm{d}\mu_\Gamma\Big\}\mathrm{d}s.
\end{aligned}
$$

Regarding (A3), (A4), (A2) and Lemma 3.2, applying the trace inequality (6.1) for $(v_i^\gamma)^{p/2}$, Hölder's, Gagliardo-Nirenberg's and Young's inequality we continue by

$$
\begin{aligned}
\mathrm{e}^{pt}\sum_{i=1}^{2}\|v_i(t)\|_{L^p}^p&\le\int_0^t\mathrm{e}^{ps}\Big\{\int_\Omega\sum_{i=1}^{2}\Big\{cp\big(u_i|\nabla z||\nabla v_i^{p-1}|+v_i^p+(\sum_{k=1}^{2}u_k+1)v_i^{p-1}\big)-\epsilon|\nabla v_i^{p/2}|^2\Big\}\mathrm{d}x\\
&\qquad\qquad+cp\sum_{\gamma=\alpha,\beta}\int_\Gamma\big((v_i^\gamma)^p+1\big)\,\mathrm{d}\Gamma\Big\}\,\mathrm{d}s\\
&\le\int_0^t\mathrm{e}^{ps}\sum_{i=1}^{2}\Big\{cp\big(\|\nabla z\|_{L^q}(\|v_i^{p/2}\|_{L^r}+1)\|v_i^{p/2}\|_{H^1}\\
&\qquad+cp\big(\|v_i^{p/2}\|_{L^2}^2+\sum_{\gamma=\alpha,\beta}\|(v_i^\gamma)^{p/2}\|_{L^2(\Gamma)}^2+1\big)-\epsilon\|v_i^{p/2}\|_{H^1}^2\Big\}\,\mathrm{d}s\\
&\le\int_0^t\mathrm{e}^{ps}\Big\{\kappa\,c\,p^{2r}\sum_{i=1}^{2}(\|v_i^{p/2}\|_{L^1}^2+1)\,\mathrm{d}s\Big\}
\end{aligned}
$$

where κ is defined in (3.10). In summary it results the estimate

$$
\sum_{i=1}^{2}\|v_i(t)\|_{L^p}^p\le cp^{2r}\kappa\sum_{i=1}^{2}\sup_{s\in S}(\|v_i(s)\|_{L^{p/2}}^p+1)\qquad\forall t\in S. \tag{3.11}
$$

Defining

$$
a_m=\sum_{i=1}^{2}\Big\{\sup_{s\in S}\|v_i(s)\|_{L^{2^m}}^{2^m}+1\Big\},\quad m=0,1,\dots
$$

the inequality (3.11) implies

$$
a_m\le c^m\,\kappa\,a_{m-1}^2\le c^{m+2(m-1)}\,\kappa^{1+2}\,a_{m-2}^4\le\dots\le c^{2^{m+1}-2-m}\,\kappa^{2^m-1}\,a_0^{2^m},
$$

and we continue estimate (3.11) by

$$
\sum_{i=1}^{2}\|v_i(t)\|_{L^{2^m}}\le c\kappa\sum_{i=1}^{2}\Big\{\sup_{s\in S}\|v_i(s)\|_{L^1}+1\Big\}.
$$

In the limit $m \to \infty$, we find

$$\sum_{i=1}^{2} \|v_i(t)\|_{L^\infty} \le c\kappa \sum_{i=1}^{2} \Big\{ \sup_{s\in S} \|v_i(s)\|_{L^1} + 1 \Big\} \qquad \forall t \in S.$$

Because of $u_i \le v_i + \widehat{K}$ the desired estimate for u_i, $i = 1, 2$, follows and then the assertion for z is a direct consequence of Lemma 3.2 ii) and the Sobolev embedding $W^{1,q}(\Omega) \hookrightarrow L^\infty(\Omega)$ for $q > 2$ in two spatial dimensions. $\square$

4 Existence and uniqueness result for (P)

4.1 A regularized problem (P_M)

In order to show the existence of solutions to (P) we study a regularized problem (P_M) defined on an arbitrarily fixed time interval $S = [0, T]$. For $M \ge M^* := \max\big\{1, \|U\|_V\big\}$ let $\rho_M : \mathbb{R}^6 \to [0, 1]$ be a Lipschitz continuous function fulfilling

$$\rho_M(u) = \begin{cases} 0 & \text{if } |u|_\infty \ge M, \\ 1 & \text{if } |u|_\infty \le M/2 \end{cases}, \qquad |u|_\infty = \max\{|u_1|, \dots, |u_{\Gamma 2}|\}.$$

Additionally, we introduce the projection

$$\sigma_M(y) := \begin{cases} -M & \text{for } \; y < -M, \\ \;\;\, y & \text{for } \; y \in [-M, M], \\ \;\;\, M & \text{for } \; y > M, \end{cases} \qquad y \in \mathbb{R},$$

and define the operators $\mathcal{A}_M \colon (X + u^D) \times (Z + z^D) \to X^*$, $\mathcal{R}_M \colon [X + u^D] \cap V_+ \to X^*$ by

$$\begin{aligned} \langle \mathcal{A}_M(u, z), \widehat{u} \rangle_X &:= \int_\Omega \sum_{i=1}^{2} D_i(\nabla u_i + \lambda_i [\sigma_M(u_i)]^+ \nabla z) \cdot \nabla \widehat{u}_i \,\mathrm{d}x, \\ \langle \mathcal{R}_M(u), \widehat{u} \rangle_X &:= \int_G \rho_M(u) \Big\{ r_1(u_1u_4 - k_1u_3)(\widehat{u}_1 + \widehat{u}_4 - \widehat{u}_3) + r_2(u_2u_3 - k_2u_4)(\widehat{u}_2 + \widehat{u}_3 - \widehat{u}_4) \Big\} \mathrm{d}\mu \\ &\quad + \sum_{\gamma=\alpha,\beta} \int_{G_\Gamma} \rho_M(u) \Big\{ r^\gamma_{\Gamma 1}(u^\gamma_1 u_{\Gamma 2} - k^\gamma_{\Gamma 1} u_{\Gamma 1})(\widehat{u}^\gamma_1 + \widehat{u}_{\Gamma 2} - \widehat{u}_{\Gamma 1}) \\ &\qquad\qquad + r^\gamma_{\Gamma 2}(u^\gamma_2 u_{\Gamma 1} - k^\gamma_{\Gamma 2} u_{\Gamma 2})(\widehat{u}^\gamma_2 + \widehat{u}_{\Gamma 1} - \widehat{u}_{\Gamma 2}) \Big\} \,\mathrm{d}\mu_\Gamma \\ &\quad + \sum_{i=1}^{2} \int_\Gamma \rho_M(u)(\sigma^\alpha_i u^\alpha_i - \sigma^\beta_i u^\beta_i)(\widehat{u}^\alpha_i - \widehat{u}^\beta_i) \,\mathrm{d}a \\ &\quad + \int_\Omega \rho_M(u) \Big\{ r_0(u_1u_2 - k_0)(\widehat{u}_1 + \widehat{u}_2) - G_{phot}(\widehat{u}_1 + \widehat{u}_2) \Big\} \,\mathrm{d}x, \quad \widehat{u} \in X. \end{aligned}$$

We study the regularized problem

$$\left.\begin{aligned} u'(t) + \mathcal{A}_M(u(t), z(t)) + \mathcal{R}_M(u^+(t)) = 0 \quad \mathcal{P}(z(t), u^+(t)) = 0, \quad \text{f.a.a. } t \in S, \\ u(0) = U,\; u \in H^1(S, X^*),\; u - u^D \in L^2(S, X),\; z - z^D \in L^2(S, Z). \end{aligned}\right\} \qquad (\mathrm{P}_M)$$

Solutions (u, z) to (P_M) fulfil $u \in C(S, Y)$ and $z - z^D \in C(S, Z)$.

4.2 Solvability of (P_M)

In this subsection the constants may depend on M and S. We work with an equivalent formulation of (P_M). We decompose u in the form $u=(v,w)$, where $v=(u_1,u_2)$, $w=(u_3,u_4,u_{\Gamma 1},u_{\Gamma 2})$ and make use of the spaces

$$Y^2=L^2(\Omega)^2,\ Y^4=L^2(G;\mathrm{d}\mu)^2\times L^2(G_\Gamma;\mathrm{d}\mu_\Gamma)^2,\ X^2=(H^1(\Omega_N^\alpha)\times H^1(\Omega_N^\beta))^2,\ X^{2*}:=(X^2)^*,$$

where $H^1(\Omega_N^\gamma):=H_0^1(\Omega\cup\Gamma_N^\gamma)$. We define operators $\mathcal{A}_v^0: L^2(S,X^2)\to L^2(S,X^{2*})$, $\mathcal{R}_v\colon (L^2(S,X^2)+v^D)\times L^2(S,Y^4)\to L^2(S,X^{2*})$, $\mathcal{A}_v\colon (L^2(S,X^2)+v^D)\times(L^2(S,Z)+z^D)\to L^2(S,X^{2*})$ and $\mathcal{R}_w\colon (L^2(S,X^2)+v^D)\times L^2(S,Y^4)\to L^2(S,Y^4)$ by

$$\begin{aligned}
\langle\mathcal{A}_v^0(v-v^D),\widehat{v}\rangle_{L^2(S,X^2)} &:= \int_S\int_\Omega\sum_{i=1}^2 D_i\nabla(v_i-v_i^D)\cdot\nabla\widehat{v}_i\,\mathrm{d}x\,\mathrm{d}s,\\
\langle\mathcal{A}_v(v,z),\widehat{v}\rangle_{L^2(S,X^2)} &:= \int_S\int_\Omega\sum_{i=1}^2 D_i(\nabla v_i^D+\lambda_i\,[\sigma_M(v_i)]^+\nabla z)\cdot\nabla\widehat{v}_i\,\mathrm{d}x\,\mathrm{d}s,\\
\langle\mathcal{R}_v(v,w),\widehat{v}\rangle_{L^2(S,X^2)} &:= \int_S\langle\mathcal{R}_M(v^+,w^+),(\widehat{v},0)\rangle_X\,\mathrm{d}s,\quad \widehat{v}\in L^2(S,X^2),\\
\langle\mathcal{R}_w(v,w),\widehat{w}\rangle_{L^2(S,Y^4)} &:= \int_S\langle\mathcal{R}_M(v^+,w^+),(0,\widehat{w})\rangle_X\,\mathrm{d}s,\quad \widehat{w}\in L^2(S,Y^4).
\end{aligned}$$

Let $v\in L^2(S,Y^2)$ and $w\in L^2(S,Y^4)$. Then $(v,w)\in L^2(S,Y)$ and by Lemma 3.1 there is a unique solution z with $z-z^D\in L^2(S,Z)\cap L^\infty(S,L^\infty(\Omega))$ of

$$\mathcal{P}(z(t),v^+(t),w^+(t))=0\quad\text{f.a.a. } t\in S.$$

By $\mathcal{T}_z\colon L^2(S,Y^2)\times L^2(S,Y^4)\to L^2(S,Z)+z^D$ we denote the corresponding solution operator such that $z=\mathcal{T}_z(v,w)$. Then the system

$$\begin{aligned}
&(v-v^D)'+\mathcal{A}_v^0(v-v^D)=-\mathcal{R}_v(v,w)-\mathcal{A}_v(v,\mathcal{T}_z(v,w)),\\
&(v-v^D)(0)=(U_1,U_2)-v^D,\quad v-v^D\in W^2,
\end{aligned}\tag{4.1}$$

$$w'+\mathcal{R}_w(v,w)=0,\quad w(0)=(U_3,U_4,U_{\Gamma 1},U_{\Gamma 2}),\quad w\in H^1(S,Y^4),\tag{4.2}$$

is an equivalent formulation of problem (P_M). Note that here

$$W^2:=\big\{v\in L^2(S,X^2)\colon v'\in L^2(S,X^{2*})\big\}\subset C(S,Y^2).$$

Solvability of (P_M) is obtained by proving that the system (4.1), (4.2) has a solution. First we give a short overview of this proof. For an arbitrarily fixed $\widehat{v}\in W^2+v^D$ we solve

$$w'+\mathcal{R}_w(\widehat{v},w)=0,\quad w(0)=(U_3,U_4,U_{\Gamma 1},U_{\Gamma 2}),\quad w\in H^1(S,Y^4),\tag{4.3}$$

and get $w=\mathcal{T}_w\widehat{v}$ with a solution operator $\mathcal{T}_w\colon W^2+v^D\to H^1(S,Y^4)$ (see Lemma 4.1). The problem

$$\begin{aligned}
(v-v^D)'+\mathcal{A}_v^0(v-v^D)&=-\mathcal{R}_v(\widehat{v},\mathcal{T}_w\widehat{v})-\mathcal{A}_v(\widehat{v},\mathcal{T}_z(\widehat{v},\mathcal{T}_w\widehat{v})),\\
(v-v^D)(0)&=(U_1,U_2)-v^D,\quad v-v^D\in W^2
\end{aligned}\tag{4.4}$$

consists of four independent linear parabolic problems for u_1^α, u_1^β, u_2^α, u_2^β and fixed given right hand sides from $L^2(S,H^1(\Omega_N^\gamma))^*$. Thus there exists a unique solution $v=\mathcal{Q}\widehat{v}$ to this problem. The operator $\mathcal{Q}$ is completely continuous (see Lemma 4.2). Using Schauder's fixed point theorem we obtain a fixed point v of $\mathcal{Q}$ (see Lemma 4.3). Then $(v,\mathcal{T}_w v)$ corresponds to a solution to (4.1), (4.2). Now we give the detailed proof.

Lemma 4.1 *We assume* (A1) – (A6). *Then for all* $\widehat{v}\in W^2+v^D$ *there is exactly one solution to* (4.3). *Moreover* $\|\mathcal{T}_w\widehat{v}\|_{C(S,Y^4)}\le c$ *for all* $\widehat{v}\in W^2+v^D$ *and*

$$\|\mathcal{T}_w\widehat{v}^1-\mathcal{T}_w\widehat{v}^2\|_{C(S,Y^4)}\le c\Big\{\|\widehat{v}^1-\widehat{v}^2\|_{L^2(S,Y^2)}+\sum_{\gamma=\alpha,\beta}\|\widehat{v}^{1\gamma}-\widehat{v}^{2\gamma}\|_{L^2(S,L^2(\Gamma)^2)}\Big\}$$

for all $\widehat{v}^1$, $\widehat{v}^2\in W^2+v^D$.

Proof. Since for $w\in L^2(S,Y^4)$ the map $w\mapsto\mathcal{R}_w(\widehat{v},w)$ is Lipschitz continuous uniformly w.r.t. $\widehat{v}$, by [7, Chapt. V, Theorem 1.3] problem (4.3) has a unique solution $w=\mathcal{T}_w\widehat{v}$ with a solution operator $\mathcal{T}_w\colon W^2+v^D\to H^1(S,Y^4)$. Since a.e. on S

$$\|\mathcal{R}_w(\widehat{v}^1,w^1)-\mathcal{R}_w(\widehat{v}^2,w^2)\|_{Y^4}\le c\Big(\|\widehat{v}^1-\widehat{v}^2\|_{Y^2}+\sum_{\gamma=\alpha,\beta}\|\widehat{v}^{1\gamma}-\widehat{v}^{2\gamma}\|_{L^2(\Gamma)^2}+\|w^1-w^2\|_{Y^4}\Big)$$

for all $(\widehat{v}^1,w^1)$, $(\widehat{v}^2,w^2)\in L^2(S,X)$ we derive by testing (4.3) (for $(\widehat{v}^1,w^1)$ and $(\widehat{v}^2,w^2)$) by w^1-w^2 and by using Gronwall's lemma the Lipschitz-estimate of Lemma 4.1. Testing (4.3) by $w=\mathcal{T}_w\widehat{v}$, taking into account that $\rho_M(u)=0$ for u with $|u|_\infty>M$ and again using Gronwall's lemma the uniform estimate for $\|\mathcal{T}_w\widehat{v}\|_{C(S,Y^4)}$ results. □

Lemma 4.2 *We assume* (A1) – (A6). *Then the mapping* $\mathcal{Q}\colon W^2+v^D\to W^2+v^D$ *is completely continuous.*

Proof. Let $\{\widehat{v}_n\}\subset W^2+v^D$ be bounded. According to [16, Theorem 5.1] and (6.1) we may assume that there exists an element $\widehat{v}\in W^2+v^D$ such that $\widehat{v}_n\to\widehat{v}$ in $L^2(S,Y^2)$, $\widehat{v}_n^\gamma\to\widehat{v}^\gamma$ in $L^2(S,L^2(\Gamma)^2)$, $\gamma=\alpha,\beta$. Let

$$v_n=\mathcal{Q}\widehat{v}_n,\ v=\mathcal{Q}\widehat{v},\ w_n=\mathcal{T}_w\widehat{v}_n,\ w=\mathcal{T}_w\widehat{v},\ z_n=\mathcal{T}_z(\widehat{v}_n,w_n),\ z=\mathcal{T}_z(\widehat{v},w).$$

Lemma 4.1 and Lemma 3.1 ensure that $w_n\to w$ in $L^2(S,Y^4)$ and $z_n-z\to 0$ in $L^2(S,Z)$. Testing (4.4) for $\widehat{v}_n$ and $\widehat{v}$ by $v_n-v\in L^2(S,X^2)$ it results

$$\begin{aligned}&\frac{1}{2}\|(v_n-v)(t)\|_{Y^2}^2+\int_0^t\epsilon\|v_n-v\|_{X^2}^2\,\mathrm{d}s\\&\le c\int_0^t\Big\{\int_\Omega\sum_{i=1}^2\Big\{|[\sigma_M(\widehat{v}_{ni})]^+-[\sigma_M(\widehat{v}_i)]^+||\nabla z|\,|\nabla(v_{ni}-v_i)|+|\nabla(z_n-z)||\nabla(v_{ni}-v_i)|\Big\}\,\mathrm{d}x\\&\qquad+\Big(\|\widehat{v}_n-\widehat{v}\|_{Y^2}+\sum_{\gamma=\alpha,\beta}\|\widehat{v}_n^\gamma-\widehat{v}^\gamma\|_{L^2(\Gamma)^2}+\|w_n-w\|_{Y^4}\Big)\|v_n-v\|_{X^2}\Big\}\,\mathrm{d}s\quad\forall t\in S.\end{aligned}$$

By Hölder's inequality and Lemma 4.1 we conclude that

$$\begin{aligned}
&\|v_n - v\|^2_{L^2(S,X^2)} \\
&\le c\|v_n - v\|_{L^2(S,X^2)}\Big\{\|\widehat{v}_n - \widehat{v}\|_{L^2(S,Y^2)} + \sum_{\gamma=\alpha,\beta}\|\widehat{v}_n^\gamma - \widehat{v}^\gamma\|_{L^2(S,L^2(\Gamma)^2)} + \|z_n - z\|_{L^2(S,Z)} \\
&\qquad + \sum_{i=1}^{2}\Big[\int_0^T\int_\Omega |[\sigma_M(\widehat{v}_{ni})]^+ - [\sigma_M(\widehat{v}_i)]^+|^2\,|\nabla z|^2\,\mathrm{d}x\,\mathrm{d}s\Big]^{1/2}\Big\}.
\end{aligned}$$

Properties of superposition operators give that the square bracket term in the last line tends to zero if $n \to \infty$. Finally we find that $v_n - v \to 0$ in $L^2(S, X^2)$. Next we estimate

$$\begin{aligned}
&\|(v_n - v)'\|_{L^2(S,X^{2*})} \\
&\le \|\mathcal{R}_v(\widehat{v}_n, w_n) - \mathcal{R}_v(\widehat{v}, w)\|_{L^2(S,X^{2*})} + \|\mathcal{A}_v^0(v_n - v)\|_{L^2(S,X^{2*})} + \|\mathcal{A}_v(\widehat{v}_n, z_n) - \mathcal{A}_v(\widehat{v}, z)\|_{L^2(S,X^{2*})} \\
&\le c\Big\{\|v_n - v\|_{L^2(S,X^2)} + \|\widehat{v}_n - \widehat{v}\|_{L^2(S,Y^2)} + \sum_{\gamma=\alpha,\beta}\|\widehat{v}_n^\gamma - \widehat{v}^\gamma\|_{L^2(S,L^2(\Gamma)^2)} + \|w_n - w\|_{L^2(S,Y^4)} \\
&\qquad + \|z_n - z\|_{L^2(S,Z)} + \sum_{i=1}^{2}\Big[\int_0^T\int_\Omega |[\sigma_M(\widehat{v}_{ni})]^+ - [\sigma_M(\widehat{v}_i)]^+|^2\,|\nabla z|^2\,\mathrm{d}x\,\mathrm{d}s\Big]^{1/2}\Big\} \to 0
\end{aligned}$$

for $n \to \infty$, and we obtain $v_n - v \to 0$ in W^2. The continuity of the operator $\mathcal{Q}$ follows by similar arguments. □

Lemma 4.3 *We assume* (A1) – (A6)*. Then there exists a fixed point of the mapping* $\mathcal{Q}$*.*

Proof. For given $\widehat{v} \in W^2 + v^D$, let $z = \mathcal{T}_z(\widehat{v}, \mathcal{T}_w\widehat{v})$ and $v = \mathcal{Q}\widehat{v}$. We use $\overline{v} := v - v^D$ as test function for (4.4), take into account (A4), (A5) and (A6) and use for $\mathcal{R}_v$ that $\rho_M(u) = 0$ if $|u|_\infty > M$ and apply (6.1), Lemma 3.1, Lemma 4.1 and Young's inequality. Then, since $\|\mathcal{T}_z(\widehat{v}, \mathcal{T}_w\widehat{v})\|_{H^1} \le c\,(1 + \|\widehat{v} - v^D\|_{Y^2})$ we find

$$\begin{aligned}
\|\overline{v}(t)\|^2_{Y^2} + \epsilon\int_0^t\|\overline{v}\|^2_{X^2}\,\mathrm{d}s &\le c + c\int_0^t\Big(1 + \|\overline{v}\|^2_{Y^2} + \sum_{\gamma=\alpha,\beta}\|\overline{v}^\gamma\|^2_{L^2(\Gamma)^2} + (1 + \|z\|_{H^1})\|\overline{v}\|_{X^2}\Big)\,\mathrm{d}s \\
&\le c + \int_0^t\big(\tfrac{\epsilon}{2}\|\overline{v}\|^2_{X^2} + c\,\big(1 + \|\overline{v}\|^2_{Y^2} + \|\widehat{v} - v^D\|^2_{Y^2}\big)\big)\,\mathrm{d}s \quad \forall t \in S.
\end{aligned}$$

Thus there is a constant $\overline{c} > 0$ such that for all $k > 0$

$$\begin{aligned}
&\mathrm{e}^{-kt}\Big(\|\overline{v}(t)\|^2_{Y^2} + \int_0^t\|\overline{v}\|^2_{X^2}\,\mathrm{d}s\Big) \\
&\le \overline{c} + \overline{c}\mathrm{e}^{-kt}\int_0^t\Big\{\Big\{\|\overline{v}\|^2_{Y^2} + \|\widehat{v} - v^D\|^2_{Y^2} + \int_0^s\big(\|\overline{v}\|^2_{X^2} + \|\widehat{v} - v^D\|^2_{X^2}\big)\,\mathrm{d}\tau\Big\}\mathrm{e}^{-ks}\mathrm{e}^{ks}\Big\}\,\mathrm{d}s \\
&\le \overline{c} + \overline{c}\mathrm{e}^{-kt}\sup_{s\in S}\Big\{\mathrm{e}^{-ks}\Big\{\|\overline{v}(s)\|^2_{Y^2} + \|\widehat{v}(s) - v^D\|^2_{Y^2} + \int_0^s\big(\|\overline{v}\|^2_{X^2} + \|\widehat{v} - v^D\|^2_{X^2}\big)\,\mathrm{d}\tau\Big\}\Big\}\frac{\mathrm{e}^{kt} - 1}{k}.
\end{aligned}$$

We take now $k \geq 3\overline{c}$ and obtain

$$\sup_{t\in S} \mathrm{e}^{-kt}\Big(\|\overline{v}(t)\|^2_{Y^2} + \int_0^t \|\overline{v}(s)\|^2_{X^2}\,\mathrm{d}s\Big)$$
$$\leq \frac{3}{2}\overline{c} + \frac{1}{2}\sup_{t\in S}\Big\{\mathrm{e}^{-kt}\Big(\|\widehat{v}(t)-v^D\|^2_{Y^2} + \int_0^t \|\widehat{v}(s)-v^D\|^2_{X^2}\,\mathrm{d}s\Big)\Big\}.$$

Once more using for the reaction terms that $\rho_M(u) = 0$ for $|u|_\infty > M$, and again applying Lemma 3.1 and Lemma 4.1 we estimate

$$\|\overline{v}'\|_{L^2(S,X^{2*})} = \sup_{\|\widetilde{v}\|_{L^2(S,X^2)}\leq 1} \langle -\mathcal{R}_v(\widehat{v},\mathcal{T}_w\widehat{v}) - \mathcal{A}^0_v(\overline{v}) - \mathcal{A}_v(\widehat{v},z),\widetilde{v}\rangle_{L^2(S,X^2)}$$
$$\leq c\,\big(\|\overline{v}\|_{L^2(S,X^2)} + \|z\|_{L^2(S,H^1)} + \|\widehat{v}-v^D\|_{L^2(S,Y^2)} + 1\big)$$
$$\leq c\,\Big(\|\overline{v}\|_{L^2(S,X^2)} + \|\widehat{v}-v^D\|_{L^2(S,Y^2)} + 1\Big)$$
$$\leq \widetilde{c}\Big(\|\overline{v}\|_{L^2(S,X^2)} + \Big[\sup_{t\in S}\Big\{\mathrm{e}^{-kt}\Big(\|\widehat{v}(t)-v^D\|^2_{Y^2} + \int_0^t \|\widehat{v}(s)-v^D\|^2_{X^2}\,\mathrm{d}s\Big)\Big\}\mathrm{e}^{kT}\Big]^{1/2} + 1\Big).$$

The non-empty, bounded, closed and convex subset of $W^2 + v^D$,

$$\mathcal{M} := \Big\{ v \in W^2 + v^D\colon \ \sup_{t\in S}\Big\{\mathrm{e}^{-kt}\Big(\|\overline{v}(t)\|^2_{Y^2} + \int_0^t \|\overline{v}\|^2_{X^2}\,\mathrm{d}s\Big)\Big\} \leq 3\overline{c},$$
$$\|\overline{v}'\|_{L^2(S,X^{2*})} \leq \widetilde{c}\,\Big(2\sqrt{3\overline{c}}\mathrm{e}^{kT} + 1\Big)\ \Big\}$$

possesses the property that $\mathcal{Q}(\mathcal{M}) \subset \mathcal{M}$. Since $\mathcal{Q}$ by Lemma 4.2 is completely continuous the assertion of Lemma 4.3 is guaranteed by Schauder's fixed point theorem. □

Theorem 4.1 *We assume assume* (A1) – (A6)*. Then there exists a solution* (u, z) *to problem* (P$_M$)*.*

Proof. Due to Lemma 4.3 there exists a solution v of the problem

$$(v - v^D)' + \mathcal{A}^0_v(v - v^D) = -\mathcal{R}_v(v,\mathcal{T}_w v) - \mathcal{A}_v(v,\mathcal{T}_z(v,\mathcal{T}_w v)),$$
$$(v - v^D)(0) = (U_1, U_2) - v^D, \quad v - v^D \in W^2.$$

Putting $w = \mathcal{T}_w v \in H^1(S, Y^4)$, the pair (v, w) fulfills the equations (4.1) and (4.2) which are an equivalent formulation of problem (P$_M$). □

4.3 Energy estimates for (P$_M$)

Lemma 4.4 *We assume* (A1) – (A6)*. Then, for any solution* (u, z) *to* (P$_M$) *and for every* $t \in S$ *the inequalities* $u_i(t) \geq 0$ *a.e. on* Ω*,* $i = 1, 2$*,* $u_i(t) \in [0, 1]$ μ*-a.e. in* G*,* $i = 3, 4$*,* $u_{\Gamma i}(t) \in [0, 1]$ μ_Γ*-a.e. in* G_Γ*,* $i = 1, 2$*, are fulfilled.*

Proof. Let (u,z) be a solution to (P_M). We use the test function $-u^-$. Taking into account that

$$\begin{aligned}
&(\nabla u_i+\lambda_i[\sigma_M(u_i)]^+\nabla z)\cdot\nabla u_i^-\le 0,\quad -G_{phot}u_i^-\le 0,\quad i=1,2,\\
&(u_1^+u_2^+-k_0)(u_1^-+u_2^-)\le 0\quad\text{a.e. on }\Omega;\\
&(u_1^+u_4^+-k_1u_3^+)(u_1^-+u_4^--u_3^-)\le 0,\\
&(u_2^+u_3^+-k_2b_4^+)(u_2^-+u_3^--u_4^-)\le 0\quad\mu\text{-a.e. on }G;
\end{aligned}$$

$$\begin{aligned}
&(u_1^{\gamma+}u_{\Gamma 2}^+-k_{\Gamma 1}u_{\Gamma 1}^+)(u_1^{\gamma-}+u_{\Gamma 2}^--u_{\Gamma 1}^-)\le 0,\\
&(u_2^{\gamma+}u_{\Gamma 1}^+-k_{\Gamma 2}u_{\Gamma 2}^+)(u_2^{\gamma-}+u_{\Gamma 1}^--u_{\Gamma 2}^-)\le 0\quad\mu_\Gamma\text{-a.e. on }G_\Gamma\quad\gamma=\alpha,\beta;\\
&(\sigma_i^\alpha u_i^{\alpha+}-\sigma_i^\beta u_i^{\beta+})(u_i^{\alpha-}-u_i^{\beta-})\le 0\quad\text{a.e. on }\Gamma,\quad i=1,2,
\end{aligned}$$

we find that $\|u^-(t)\|_Y^2\le 0$ for all $t\in S$. We argue now as in the proof of Lemma 3.2 to verify the remaining results of the lemma. $\square$

We work with a regularized free energy functional F_M^0 which is compatible with the regularizations done in problem (P_M). Let δ fulfill (3.6). Writing for quantities y the expression $y^\delta:=\max\{y,\delta\}$ and using the function

$$l_M(y)=\begin{cases}\ln y & \text{if}\quad 0<y\le M,\\ \ln M-1+\frac{y}{M} & \text{if}\quad y>M,\end{cases}$$

we introduce the functionals $\widetilde{F}_{M2}^\delta:Y\to\overline{\mathbb{R}}$ by

$$\begin{aligned}
\widetilde{F}_{M2}^\delta(u)=&\int_\Omega\sum_{i=1}^2\int_{u_i^D}^{u_i}(l_M(y^\delta)-\ln u_i^D)\,\mathrm{d}y\,\mathrm{d}x+\sum_{i=3}^4\int_G\int_{\widetilde{u}_i}^{u_i}(l_M(y^\delta)-\ln\widetilde{u}_i)\,\mathrm{d}y\,\mathrm{d}\mu\\
&+\sum_{i=1}^2\int_{G_\Gamma}\int_{\widetilde{u}_{\Gamma i}}^{u_{\Gamma i}}(l_M(y^\delta)-\ln\widetilde{u}_{\Gamma i})\,\mathrm{d}y\,\mathrm{d}\mu_\Gamma\quad\text{if }u\in Y_+,
\end{aligned}$$

and $\widetilde{F}_{M2}^\delta(u)=+\infty$ for $u\in Y\setminus Y_+$. Additionally, we set

$$F_{M2}^\delta=(\widetilde{F}_{M2}^{\delta*}|_X)^*:X^*\to\overline{\mathbb{R}},\quad F_M^\delta=F_1+F_{M2}^\delta:X^*\to\overline{\mathbb{R}},$$

with F_1 from Subsection 3.1. Note that the function l_M has the same essential properties as the ln-function occurring in the definition of F_2 and that for $u\in Y$ we have $F_{M2}^\delta(u)\to F_{M2}^0(u)$ and $F_M^\delta(u)\to F_M^0(u)$ as $\delta\downarrow 0$, where $F_{M2}^0(u)$ means $F_{M2}^\delta(u)$ for $\delta=0$. Especially, by the definition of F_1 and l_M we have for $u\in Y_+$ and z with $\mathcal{P}(z,u)=0$ that

$$\|z-z^D\|_Z^2,\ \|u_i\ln u_i\|_{L^1},\ \|u_i\|_{L^1}\le cF_M^0(u)+\widetilde{c},\quad i=1,2.\tag{4.5}$$

Lemma 4.5 *We assume* (A1)–(A6). *Let* (u,z) *be a solution to* (P_M) *and* $u^\delta=\max\{u,\delta\}$ *for* $\delta<M$ *fulfilling* (3.6). *Then for all* $\tau>0$ *there exist constants* $c_\tau>0$, $c>0$

(*independently on M and δ*) *such that*

$$\int_0^t \sum_{\gamma=\alpha,\beta} \Big\{ \|\rho_M(u^\delta) r^\gamma_{\Gamma 1}(u^\gamma_1)^\delta (u_{\Gamma 2})^\delta\|_{L^1(G_\Gamma, \mathrm{d}\mu_\Gamma)} + \|\rho_M(u^\delta) r^\gamma_{\Gamma 2}(u^\gamma_2)^\delta (u_{\Gamma 1})^\delta\|_{L^1(G_\Gamma, \mathrm{d}\mu_\Gamma)} \Big\} \,\mathrm{d}s$$
$$\leq c + \int_0^t \Big\{ \sum_{i=1}^2 \Big\{ \tau \int_\Omega \sigma_M(u_i^\delta)|\nabla l_M(u_i^\delta) + \lambda_i \nabla z|^2 \,\mathrm{d}x + c_\tau \|u_i^\delta\|_{L^1(\Omega)} + c\|\nabla(u_i - u_i^\delta)\|_{L^1} \Big\}$$
$$+ c(1 + M\delta + \delta^2) \Big\} \,\mathrm{d}s \quad \forall t > 0.$$

Proof. According to Lemma 4.4 we have $u \geq 0$ for solutions to (P_M). Similar to the proof of Lemma 3.3, testing in (P_M) the equations for u_i, $i = 1, 2$, on Ω^α by ϕ^α, adding them and leaving out nonnegative terms on the left hand side we here obtain

$$\int_0^t \Big\{ \int_{G_\Gamma} \rho_M(u)(r^\alpha_{\Gamma 1} u^\alpha_1 u_{\Gamma 2} + r^\alpha_{\Gamma 2} u^\alpha_2 u_{\Gamma 1}) \,\mathrm{d}\mu_\Gamma + \sum_{i=1}^2 \int_\Gamma \rho_M(u)(\sigma^\alpha_i u^\alpha_i - \sigma^\beta_i u^\beta_i) \,\mathrm{d}a \Big\} \,\mathrm{d}s$$
$$\leq \sum_{i=1}^2 \Big\{ \|U_i\|_{L^1(\Omega^\alpha)} + \int_0^t \Big\{ c + \int_{\Omega^\alpha} \frac{D_i}{\kappa_0} |\nabla u_i + \lambda_i \sigma_M(u_i) \nabla z| \,\mathrm{d}x \Big\} \,\mathrm{d}s \Big\} \quad \forall t \in S.$$

Because of $\rho_M(u) = 0$ for $|u|_\infty \geq M$ we find

$$\rho_M(u^\delta)\big[(u^\gamma_1)^\delta (u_{\Gamma 2})^\delta + (u^\gamma_2)^\delta (u_{\Gamma 1})^\delta\big] \leq \rho_M(u)\big[u^\gamma_1 u_{\Gamma 2} + u^\gamma_2 u_{\Gamma 1}\big] + c(M\delta + \delta^2).$$

Since $\sigma_M(u^\delta) = \sigma_M(u)$ and $\nabla u_i^\delta = \sigma_M(u_i^\delta)\nabla l_M(u_i^\delta)$ we estimate the drift-diffusion term finally using Young's inequality and $\sigma_M(u_i^\delta) \leq u_i^\delta$ by

$$\begin{aligned} |\nabla u_i + \lambda_i \sigma_M(u_i) \nabla z| &\leq |\nabla u_i^\delta + \lambda_i \sigma_M(u_i^\delta) \nabla z| + |\nabla(u_i^\delta - u_i)| \\ &\leq \sigma_M(u_i^\delta)|\nabla l_M(u_i^\delta) + \lambda_i \nabla z| + |\nabla(u_i^\delta - u_i)| \\ &\leq \tau \sigma_M(u_i^\delta)|\nabla l_M(u_i^\delta) + \lambda_i \nabla z|^2 + c_\tau |u_i^\delta| + c|\nabla(u_i - u_i^\delta)|. \end{aligned}$$

This together leads to

$$\int_0^t \Big\{ \|\rho_M(u^\delta) r^\alpha_{\Gamma 1}(u^\alpha_1)^\delta (u_{\Gamma 2})^\delta\|_{L^1(G_\Gamma, \mathrm{d}\mu_\Gamma)} + \|\rho_M(u^\delta) r^\alpha_{\Gamma 2}(u^\alpha_2)^\delta (u_{\Gamma 1})^\delta\|_{L^1(G_\Gamma, \mathrm{d}\mu_\Gamma)}$$
$$+ \sum_{i=1}^2 \int_\Gamma \rho_M(u)(\sigma^\alpha_i u^\alpha_i - \sigma^\beta_i u^\beta_i) \,\mathrm{d}a \Big\} \,\mathrm{d}s$$
$$\leq c + \int_0^t \Big\{ \sum_{i=1}^2 \Big\{ \tau \int_\Omega \sigma_M(u_i^\delta)|\nabla l_M(u_i^\delta) + \lambda_i \nabla z|^2 \,\mathrm{d}x + c_\tau \|u_i^\delta\|_{L^1(\Omega)} + c\|\nabla(u_i - u_i^\delta)\|_{L^1} \Big\}$$
$$+ c(1 + M\delta + \delta^2) \Big\} \,\mathrm{d}s \quad \forall t \in S.$$

Similar results are obtained by testing the equations for u_i, $i = 1, 2$, on Ω^β by ϕ^β, only the term $\int_\Gamma \rho_M(u)(\sigma^\alpha_i u^\alpha_i - \sigma^\beta_i u^\beta_i) \,\mathrm{d}a$ then has the opposite sign. Combining both estimates, the assertion of the lemma follows. $\square$

Lemma 4.6 *Under the assumptions* (A1) – (A6) *there exist constants* $c_1(T)$, $c_2(T) > 0$ *not depending on* M *such that*

$$F_M^0(u(t)) \le c_1(T), \quad \|u_i(t)\ln u_i(t)\|_{L^1} \le c_2(T), \quad i=1,2, \quad \forall t \in S$$

for any solution (u,z) *to* (P_M).

Proof. Let (u,z) be a solution to (P_M), let $\delta < M$ fulfill (3.6), and let $u^\delta = \max\{u,\delta\}$. Then $u \in H^1(S,X^*)$, $u \ge 0$, $z - z^D \in L^2(S,Z)$,

$$w_M^\delta := \Big(\big(l_M(u_i^\delta) - \ln u_i^D\big)_{i=1,2}, \big(l_M(u_i^\delta) - \ln \widetilde{u}_i\big)_{i=3,4}, \big(l_M(u_{\Gamma i}^\delta) - \ln \widetilde{u}_{\Gamma i}\big)_{i=1,2}\Big) \in L^2(S,X),$$

and $\lambda(z(t)-z^D) \in \partial F_1(u(t))$, $w_M^\delta(t) \in \partial F_{M2}^\delta(u(t))$ f.a.a. $t \in S$ (note that $l_M(u_i^\delta) = \ln u_i^D$ a.e. on $S \times \Gamma_D$, $i=1,2$, and by Lemma 4.4 we have $l_M(u_i^\delta) = \ln u_i^\delta$, $i=3,4$, $l_M(u_{\Gamma i}^\delta) = \ln(u_{\Gamma i}^\delta)$, $i=1,2$). Thus, according to Lemma 6.1, we get for $\zeta_M^\delta := w_M^\delta + \lambda(z-z^D)$ that

$$\begin{aligned}
\Big[F_1(u(t)) + F_{M2}^\delta(u(t))\Big]\Big|_0^t &= \int_0^t \langle u'(s), \zeta_M^\delta(s)\rangle_X \,\mathrm{d}s \\
&= -\int_0^t \langle \mathcal{R}_M(u(s)) + \mathcal{A}_M(u(s),z(s)), \zeta_M^\delta(s)\rangle_X \,\mathrm{d}s \\
&= -\int_0^t \big\{\langle \mathcal{R}_M(u^\delta(s)) + \mathcal{A}_M(u^\delta(s),z(s)), \zeta_M^\delta(s)\rangle_X - \theta^\delta(s)\big\}\,\mathrm{d}s,
\end{aligned}$$

where $\theta^\delta = \langle \mathcal{R}_M(u^\delta) - \mathcal{R}_M(u) + \mathcal{A}_M(u^\delta,z) - \mathcal{A}_M(u,z), \zeta_M^\delta\rangle_X \to 0$ for $\delta \downarrow 0$. Since all the reaction terms containing the factor $\rho_M(u^\delta)$ become zero if $|u^\delta|_\infty > M$, we have for these terms only to discuss the situation $u_i^\delta \le M$, and here is $l_M(u_i^\delta) = \ln u_i^\delta$. We arrive at

$$\begin{aligned}
-\langle \mathcal{R}_M(u^\delta), \zeta_M^\delta\rangle_X \le{}& c\,(1 + \sum_{i=1}^2 \|u_i^\delta\|_{L^1})\Big(\|\ln \tfrac{u_1^D u_2^D}{k_0}\|_{L^\infty} + \|\tfrac{k_1k_2}{u_1^D u_2^D}\|_{L^\infty(G,\mathrm{d}\mu)}\Big) \\
&+ c\,\|G_{phot}\|_{L^\infty}\Big\{\sum_{i=1}^2 \big(\|u_i^\delta\|_{L^1} + \|\ln u_i^D\|_{L^1}\big) + \|z - z^D\|_{L^1}\Big\} \\
&+ c\,(1 + \|\rho_M(u^\delta) r_{\Gamma 1}^\beta (u_1^\beta)^\delta (u_{\Gamma 2})^\delta\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)})\|\tfrac{k_{\Gamma 1}^\beta u_1^{\alpha D}}{k_{\Gamma 1}^\alpha u_1^{\beta D}}\|_{L^\infty(G_\Gamma,\mathrm{d}\mu_\Gamma)} \\
&+ c\,(1 + \|\rho_M(u^\delta) r_{\Gamma 2}^\alpha (u_2^\alpha)^\delta (u_{\Gamma 1})^\delta\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)})\|\tfrac{k_{\Gamma 1}^\alpha k_{\Gamma 2}^\alpha}{u_1^{\alpha D} u_2^{\alpha D}}\|_{L^\infty(G_\Gamma,\mathrm{d}\mu_\Gamma)} \\
&+ c\,(1 + \|\rho_M(u^\delta) r_{\Gamma 2}^\beta (u_2^\beta)^\delta (u_{\Gamma 1})^\delta\|_{L^1(G_\Gamma,\mathrm{d}\mu_\Gamma)})\|\tfrac{k_{\Gamma 1}^\alpha k_{\Gamma 2}^\beta}{u_1^{\alpha D} u_2^{\beta D}}\|_{L^\infty(G_\Gamma,\mathrm{d}\mu_\Gamma)}.
\end{aligned}$$

Having in mind that on solutions $[\sigma_M(u_i^\delta)]^+ = \sigma_M(u_i^\delta) \le u_i^\delta$, $\nabla l_M(u_i^\delta) = \nabla(u_i^\delta)/\sigma_M(u_i^\delta)$, $i=1,2$, using (A4), (A5) and Young's inequality we find

$$\begin{aligned}
&-\langle \mathcal{A}_M(u^\delta,z), \zeta_M^\delta\rangle_X \\
&= -\int_\Omega \sum_{i=1}^2 D_i \sigma_M(u_i^\delta)\Big\{|\nabla(l_M(u_i^\delta) + \lambda_i z)|^2 - \nabla(l_M(u_i^\delta) + \lambda_i z)\cdot\nabla(\ln u_i^D - \lambda_i z^D)\Big\}\,\mathrm{d}x \\
&\le \sum_{i=1}^2 \Big(c\|u_i^\delta\|_{L^1}\|\nabla(\ln u_i^D + \lambda_i z^D)\|_{L^\infty}^2 - \tfrac{\epsilon}{2}\int_\Omega \sigma_M(u_i^\delta)|\nabla(l_M(u_i^\delta) + \lambda_i z)|^2\,\mathrm{d}x\Big) \quad \text{a.e. on } S.
\end{aligned}$$

Putting both estimates together, using Lemma 4.5, taking $\delta \downarrow 0$ in the previous three estimates and using (A3), (A5) and (4.5) we arrive at

$$F_M^0(u(t)) - F_M^0(U) \le c\int_0^t (1 + F_M^0(u(s)))\,\mathrm{d}s,$$

where c depends on the data, but not on M. Due to the choice of M we have $F_M^0(U) = F(U)$. By Gronwall's lemma we obtain the first assertion of the lemma, and the last result of the lemma follows by (4.5). □

4.4 Further estimates for (P_M)

Theorem 4.2 *Under the assumptions* (A1) – (A6) *there is a constant* $c^*(T) > 0$ *not depending on* M *such that for any solution* (u, z) *to* (P_M)

$$\|u\|_{L^\infty(S,V)} \le c^*(T). \tag{4.6}$$

Proof. 1. Let $q > 2, r$ and r' be chosen as in Lemma 3.2 ii) and (3.3) and let (u, z) be a solution to (P_M). By Lemma 4.4 and Lemma 3.2 ii) it results

$$\|z(t)\|_{W^{1,q}} \le c\Big[1 + \textstyle\sum_{i=1,2}\|u_i(t)\|_{L^{r'}}\Big] \quad \forall t \in S. \tag{4.7}$$

2. Let $v_i = (u_i - \widehat{K})^+$, $i = 1, 2$, where $\widehat{K}$ is given in (3.8). We test (P_M) by $2(v_1, v_2, 0, 0, 0, 0)$. Estimating $[\sigma_M(u_i)]^+$ by $v_i + \widehat{K}$, using Lemma 4.4, (4.7), (6.2), the trace inequality (6.1), Young's inequality, Lemma 4.6 and (4.5) we obtain

$$\begin{aligned}\sum_{i=1,2}\|v_i(t)\|_{L^2}^2 &\le \int_0^t \sum_{i=1,2}\Big\{ -2\epsilon\|v_i\|_{H^1}^2 + c(\|v_i\|_{L^r}\|z\|_{W^{1,q}}\|v_i\|_{H^1} + \|z\|_{H^1}\|v_i\|_{H^1} \\ &\qquad + \|v_i\|_{L^2}^2 + \sum_{\gamma=\alpha,\beta}\|v_i^\gamma\|_{L^2(\Gamma)}^2 + 1)\Big\}\,\mathrm{d}s \\ &\le \int_0^t \sum_{i=1,2}\Big\{ -\epsilon\|v_i\|_{H^1}^2 + \overline{c}\|v_i\|_{L^r}\|v_i\|_{H^1}\sum_{k=1,2}\|v_k\|_{L^{r'}} + c\Big\}\,\mathrm{d}s.\end{aligned}$$

By $\|v_k\|_{L^{r'}} \le \|v_k\|_{L^1}^{(r-2)/r}\|v_k\|_{L^2}^{2/r}$, by inequality (6.3) for $p = 2$ and by Lemma 4.6 we get

$$\begin{aligned}\overline{c}\sum_{i=1,2}\|v_i\|_{L^r}\|v_i\|_{H^1}\sum_{k=1,2}\|v_k\|_{L^{r'}} &\le \sum_{i=1,2}\Big\{\frac{\epsilon}{2}\|v_i\|_{H^1}^2 + c\|v_i\|_{L^2}^2\sum_{k=1,2}\|v_k\|_{L^2}^2\Big\} \\ \le \sum_{i=1,2}\Big\{\frac{\epsilon}{2}\|v_i\|_{H^1}^2 + \Big[\frac{\sqrt{\epsilon}}{2c_2(T)}\|v_i\ln v_i\|_{L^1}\|v_i\|_{H^1} + c\|v_i\|_{L^1}\Big]^2\Big\} &\le \sum_{i=1,2}\epsilon\|v_i\|_{H^1}^2 + c.\end{aligned}$$

By the previous estimates and inequality (4.7) we find positive constants $c(T)$, $\widetilde{\kappa}$ independent of M such that

$$\|v_i(t)\|_{L^2} \le c(T)\,,\ i = 1, 2, \quad \|z(t)\|_{W^{1,q}}^{2r} + 1 \le \widetilde{\kappa}(T) \quad \forall t \in S. \tag{4.8}$$

3. Similar to the estimates in the proof of Theorem 3.2, but estimating $[\sigma_M(u_i)]^+$ by $v_i + \widehat{K}$ and using $\widetilde{\kappa}(T)$ from (4.8) instead of κ we can verify that $\|v_i(t)\|_{L^\infty} \le c(T)$ for all $t \in S$ which leads to the desired upper bounds for u_i, $i = 1, 2$, on S. Since by Lemma 4.4 the quantities u_3, u_4, $u_{\Gamma 1}$ and $u_{\Gamma 2}$ lie in $[0, 1]$ for all $t \in S$, the proof is done. □

4.5 Existence and uniqueness result for (P)

Theorem 4.3 *We assume* (A1) – (A6). *Then there exists at least one solution to* (P).

Proof. Note that it is sufficient to show the existence of a solution to (P) on any finite time interval $S = [0, T]$. We call such problems (P_S) and choose the regularization level $\overline{M} = 2\,c^*(T)$ (see Theorem 4.2). Then Theorem 4.1 guarantees a solution (u, z) to $(\mathrm{P}_{\overline{M}})$. The choice of $\overline{M}$ ensures that the operators $\mathcal{R}_{\overline{M}}$ and $\mathcal{R}$ as well as the operators $\mathcal{A}_{\overline{M}}$ and $\mathcal{A}$ coincide on this solution. Therefore (u, z) is a solution to (P_S), too. □

Theorem 4.4 *Under the assumptions* (A1) – (A6) *the solution to* (P) *is unique.*

Proof. We prove uniqueness on every finite time interval $S := [0, T]$. Let (u^k, z^k), $k = 1, 2$, be two solutions to (P). We find a constant $c > 0$ such that $\|u^k(t)\|_V$, $\|\nabla z^k(t)\|_{L^q} \le c$ f.a.a. $t \in S$, $k = 1, 2$, where $q > 2$ (see Lemma 3.2 ii), too). Let $\overline{u} := u^1 - u^2$, $\overline{z} := z^1 - z^2$. According to (3.1) we obtain

$$\|\overline{z}(t)\|_{H^1} \le c\|\overline{u}(t)\|_Y \quad \text{f.a.a. } t \in S. \tag{4.9}$$

We test (P) by $\overline{u} \in L^2(S, X)$ and take into account Lemma 3.2 i) and the fact that the reaction rates are uniformly locally Lipschitz continuous in the state variable. With the Gagliardo-Nirenberg inequality $\|\overline{u}_i\|_{L^r(\Omega^\gamma)} \le \|\overline{u}_i\|^{2/r}_{L^2(\Omega^\gamma)} \|\overline{u}_i\|^{1-2/r}_{H^1(\Omega^\gamma)}$, $i = 1, 2$, $\gamma = \alpha, \beta$, for r from (3.3), with inequality (4.9), the trace inequality (6.1) for $\|\overline{u}_i^\gamma\|^2_{L^2(\Gamma)}$ and with Young's inequality we conclude as follows

$$\begin{aligned}
&\tfrac{1}{2}\|\overline{u}(t)\|^2_Y + \sum_{i=1,2} \int_0^t \epsilon \|\overline{u}_i\|^2_{H^1} \mathrm{d}s \\
&\le c \int_0^t \Big\{ \sum_{i=1}^{2} \Big\{ \|\overline{u}_i\|_{L^r} \|\nabla z^1\|_{L^q} \|\nabla \overline{u}_i\|_{L^2} + \|\nabla \overline{z}\|_{L^2} \|\nabla \overline{u}_i\|_{L^2} + \sum_{\gamma=\alpha,\beta} \|\overline{u}_i^\gamma\|^2_{L^2(\Gamma)} \Big\} + \|\overline{u}\|^2_Y \Big\} \mathrm{d}s \\
&\le \int_0^t \Big\{ \sum_{i=1}^{2} \Big\{ \tfrac{\epsilon}{4} \|\overline{u}_i\|^2_{H^1} + c\|\overline{u}_i\|^{2/r}_{L^2} \|\nabla z^1\|_{L^q} \|\overline{u}_i\|^{2-2/r}_{H^1} \Big\} + c\|\overline{u}\|^2_Y \Big\} \mathrm{d}s \\
&\le \int_0^t \Big\{ \sum_{i=1}^{2} \Big\{ \tfrac{\epsilon}{2} \|\overline{u}_i\|^2_{H^1} + c\|\nabla z^1\|^r_{L^q} \|\overline{u}_i\|^2_{L^2} \Big\} + c\|\overline{u}\|^2_Y \Big\} \mathrm{d}s \\
&\le \int_0^t \Big\{ \sum_{i=1}^{2} \tfrac{\epsilon}{2} \|\overline{u}_i\|^2_{H^1} + c\|\overline{u}\|^2_Y \Big\} \mathrm{d}s \quad \forall t \in S.
\end{aligned}$$

Therefore Gronwall's lemma leads to $\overline{u} = 0$ on S, and (4.9) completes the proof. □

5 Remarks and generalizations of the results of the paper

1. In the paper we studied the simplest situation of a heterostructure Ω with active interface as indicated in Figure 1 consisting of two materials Ω^α and Ω^β and an active interface

Γ in between. The presented results can easily be generalized to the situation of multi-material-heterostructures with several active interfaces. But for the analytic treatment we need that active interfaces and the parts of the boundary of Ω, where Dirichlet boundary conditions are prescribed, are strictly separated (see Lemma 3.3 and Lemma 4.5).

2. In our paper we restricted for an easier writing to the case of exactly one kind of traps in the volume and one kind of traps at the interface. The results of the paper remain true, if different kinds of traps (in possibly different subdomains) and different kinds of traps on interfaces are considered. Such models are presented in [20], there also the 1D simulation tool AFORS-HET for the simulation of solar cells and solar cell characterization methods are introduced. Especially in solar cells with polycrystalline materials there occur simultaneously acceptor like and donator like traps at grain boundaries which have Gaussian like profiles with respect to their energy distribution where both profiles are slightly shifted against each other.

3. Of course also volume or interface traps which can be occupied by multiple charge carriers can be treated by our technique. We would have to use then charge numbers appropriate for this situation and we would have to introduce additional ionization reactions.

4. In [11] we presented a (formal) generalized gradient flow formulation for electro-reaction-diffusion systems on heterostructures and with active interfaces. This paper is an extension of the ideas in [17] to heterostructures and to active interfaces, where at interfaces the following effects are taken into account: drift-diffusion processes and reactions of species living on the interface and transfer mechanisms allowing bulk species to pass the interface.

For the case of closed systems the equations discussed in the present paper can be written as a generalized gradient flow, too, provided that the rate coefficients of the generation/recombination of electrons and holes k_0, of the bulk ionization reactions k_i, of the ionization reactions at the interface $k^\gamma_{\Gamma i}$ and the coefficients σ_i^γ in the thermionic emission interface condition, $i = 1, 2$, $\gamma = \alpha, \beta$, fulfill Wegscheider conditions allowing for detailed balance of the reactions under consideration. Have in mind that in our notation the transfer coefficients σ_i^γ are incorporated in the boundary value functions $u_i^{\gamma D}$ (see assumption (A5)).

6 Appendix

Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitzian domain. We use Sobolev's imbedding results (see [15]) and the following trace inequality which can be derived from [15, p. 317, equ. 5] by a modified application of Hölder's inequality

$$\|w\|^q_{L^q(\partial\Omega)} \le c_\Omega\, q \|w\|^{q-1}_{L^{2(q-1)}(\Omega)} \|w\|_{H^1(\Omega)} \quad \forall w \in H^1(\Omega), \quad q \ge 2. \tag{6.1}$$

Moreover, we take advantage of the Gagliardo-Nirenberg inequality

$$\|w\|_{L^p} \le c_p \,\|w\|^{1/p}_{L^1} \|w\|^{1-1/p}_{H^1} \quad \forall w \in H^1(\Omega)\,,\ 1 < p < \infty \tag{6.2}$$

(see [4, 19]). As an extended version of this inequality one obtains that for any $\delta > 0$ and any $p \in (1,\infty)$ there exists a $c_{\delta,p} > 0$ such that

$$\|w\|^p_{L^p} \le \delta \,\|w \ln |w|\|_{L^1} \,\|w\|^{p-1}_{H^1} + c_{\delta,p} \,\|w\|_{L^1} \quad \forall w \in H^1(\Omega). \tag{6.3}$$

This inequality is verified in [1] for bounded smooth domains and $p = 3$. But (6.3) is true for bounded Lipschitzian domains and $p \in (1, \infty)$, too, since (6.2) is valid in this situation, too. Finally, we make use of the following chain rule, which can be derived from [2, Lemma 3.3].

Lemma 6.1 *Let X be a Hilbert space, X^* its dual, $S = [0, T]$. Let $F : X^* \to \overline{\mathbb{R}}$ be proper, convex and semicontinuous. Assume that $u \in H^1(S, X^*)$, $f \in L^2(S, X)$ and $f(t) \in \partial F(u(t))$ f.a.a. $t \in S$. Then $F \circ u : S \to \mathbb{R}$ is absolutely continuous, and*

$$\frac{\mathrm{d}\, F \circ u}{\mathrm{d}t}(t) = \Big\langle \frac{\mathrm{d}u}{\mathrm{d}t}(t), f(t) \Big\rangle_X \quad \text{f.a.a. } t \in S.$$

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